KolXPD

1 General information

1.1 Author

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1.2 Purpose

KolXPD is a multi-purpose software for photoelectron spectroscopy data measurement and processing. It was originally developed for the data acquisition using Omicron EA125 and Specs Phoibos 150 hemispherical electron analysers at the Department of Surface and Plasma Science at the Charles University in Prague. Consequently, its functionality was extended to control of other hardware, e.g. manipulator for azimuthal and polar rotation of the sample or monochromator of the Materials Science Beamline at the Elettra synchrotron in Trieste. Sophisticated and customizable import and fitting modules permit to use KolXPD also for advanced data processing of any spectroscopic data acquired on other hardware.

1.3 Features

- focused to photoelectron spectroscopy (data acquisition and processing)
- very fast data viewing and processing (complex fitting module)
- energy- and angle-resolved experiments (hardware control of commercial and custom-made experimental equipment – energy analyzers, sample manipulators, beamline monochromators...)
- import and export of variety file formats
- handling of huge amount of data
- fitting, overlay and waterfall charts, quantitative preview using the built-in database of photoionization cross sections and analyzer transmission function
- functionality customizable on request

1.4 Installation and activation

1.4.1 Installation

- Download KolXPD setup from http://kolxpd.kolibrik.net.
- Execute setup file, it will guide you through installation process.
- You can run KolXPD now, plain installation of KolXPD works as data viewer without activation.

1.4.2 Activation of a license

- If you purchased a license, you were supplied by a license file. Find this file and prepare for opening in activation process.
- Run KolXPD and click on the button "Registration ..." in the about panel in the middle, it will open licensing window.
- Click the button "Enter license file ...". It will open your internet browser with a registration form.

- Enter a license file here and submit the form. Activation file will be generated and sent to your email.
- Open your email and save attached activation file anywhere temporarily.
- In license window of KolXPD click the button "Enter activation file ...", find the activation file and open it.
- KolXPD will be activated and the "about" panel will change and show your license information.

1.4.3 Creating a trial license

- Install and run KolXPD and then click on the button "Registration ..." in the about panel in the middle, it will open licensing window.
- Click the button "Generate trial license ...". It will open your internet browser with a registration form.
- Fill in the form and submit. Trial license will be generated and activation file will be sent you by email.
- Follow 5th point of "Activation of a license".

1.4.4 Remarks about the activation

- Activation must be done by Windows user account that has rights to install (e.g. same user that installed KolXPD).
- Activation works for all Windows user accounts.
- Activation file must be used exactly for that computer, from which it was generated.
- With one license you can activate only one KolXPD installation at a time.
- If you need to reinstall computer or you move to new one, you can activate KolXPD using a license file again.
- Standard activation needs internet connection. If your computer does not have connection, select offline activation procedure in licensing window and follow instructions. You will need other computer with internet connection and a flash disk to transfer files between computers.
- After activation you can delete the activation file. You should keep your license files. The authors keeps all license files backed up, in case you lose them just contact him.

1.4.5 Configuration

If KolXPD is used only for data processing but not acquisition there is no need to modify any file!
For currently used hardware control following must be present:

- Specs Phoibos 150 electron analyzer:
  SpecsLab2 must be properly installed and working. SL2_AD.dll file (supplied by Specs) must be copied to the program directory (usually C:\Program Files\KolXPD).
  - In Trieste (1D-DLD detector):
    The defaults.ini file located in the user directory (usually C:\Documents and Settings\[user]\Application Data\kolibrik.net\KolXPD) must contain the following section with multiplier energy calibration file:
    ```
    [Phoibos]
    ```

```
DLD1DCalibrationFile=c:\Program
Files\SPECS\SpecsLab2\database\datasetCalib
1d\phoibos150-DLD1D.calib1d
```

- In Prague (MCD9 detector):
  The defaults.ini file located in the user directory (usually C:\ Documents and Settings\[user]\Application Data\kolibrik.net\KolXPD) must contain the following section with multiplier energy dispersion factors:

```
[Phoibos]
Channel_1_Delta=-0.11155    (use
Channel_2_Delta=-0.08419    correct
Channel_3_Delta=-0.05706    numbers)
Channel_4_Delta=-0.03011
Channel_5_Delta=-0.00338
Channel_6_Delta= 0.02302
Channel_7_Delta= 0.04880
Channel_8_Delta= 0.07471
Channel_9_Delta= 0.10158
```

- Sample manipulator in Trieste:
  MotorControl must be properly installed and working.
  The defaults.ini file located in the user directory (usually C:\ Documents and Settings\[user]\Application Data\kolibrik.net\KolXPD) must contain the following section:

```
[Manipulator]
type=MSB
COM=COM5                (COM port number)
COMBAUD=57600           (baudrate of the COM port)
ForceAzSlow=true        (move azimuth slowly)
ForcePolSlow=false      (move azimuth fast)
Az_Max=95               (azimuth
Az_Min=-95              and polar
Pol_Max=90              angle
Pol_Min=-25             limits
AzStep_Min=0.1          and minimum
PolStep_Min=0.05        steps)
```

- Sample manipulator in Prague:
  ???
- Beamline monochromator in Trieste:
  The defaults.ini file must contain the following section:

```
[Monochromator]
Simulation=false        (use true for testing)
Host=192.168.16.2       (IP address if connected through TCP)
#host=COM4              (COM port if connected through serial)
Port=20005              (TCP port)
COMBAUD=9600            (COM baudrate)
E_min=21.2              (photon energy
E_max=1001              limits and
energyEpsilon=0.04      minimum step)
```

1.5 File types

1.5.1 Open

KolXPD can directly open following files (usually recognized automatically from the extension or content):

xps:	single photoemission region;
xpd:	photon energy, angular and sequence scans (see 2.4.1);
exp:	complete experimental file that may contain regions, scans and folders of them;
xml:	full (i.e. non-compacted) SpecsLab2 datafiles containing groups and regions, separated channel and sweep data are then available for browsing and export;
xy:	xy files exported from SpecsLab2 (summed channel and sweep data);
dat, txt:	text files containing at column(s) of data; 2 columns are treated as energy-intensity pairs, if only 1 or more than 2 columns are found Import dialog appears (see 4.1.3);
itx:	Igor Text files;
cls:	cluster file for EDAC XPD pattern calculations;
pd:	result of EDAC calculated XPD pattern. 2D angle data, each angle point contains only a number - calculated intensity;
1,2,3...	DAT125 datafiles obtained from Spectra/WSpectra acquisition software;
spe:	Scienta datafiles;
are:	???;

Omicron DAT???.

1.5.2 Save

KolXPD can save the data in following files described in 1.5.1: exp, xpd, xps. Other opened files can be saved only in these formats. All separated channel and sweep data (if present) are summed together in each region (analogously to the "Compact Data" function in SpecsLab2.

1.5.3 Import

There is a special dialog for importing the data acquired with the VG 2D-detector data described in 4.1.5.

1.5.4 Export

All sequenced data (e.g. acquired or fitted curves, fit parameters evolution) can be exported into single or multiple text files (txt, dat, itx etc.) of preferred single- or multi-column structure. Images (graphs, plots etc.) can be exported in bmp, wmf and emf formats.

1.5.5 Clipboard

Similarly to 1.5.4 all regions, folders, scans, data and images can be copied to Windows Clipboard™ and then pasted in KolXPD, Microsoft Office™ documents and other supported programs. The data from other programs can be also pasted from Windows Clipboard™ into KolXPD; depending on the data in the clipboard the Import dialog can appear (see 4.1.3).

2 User interface

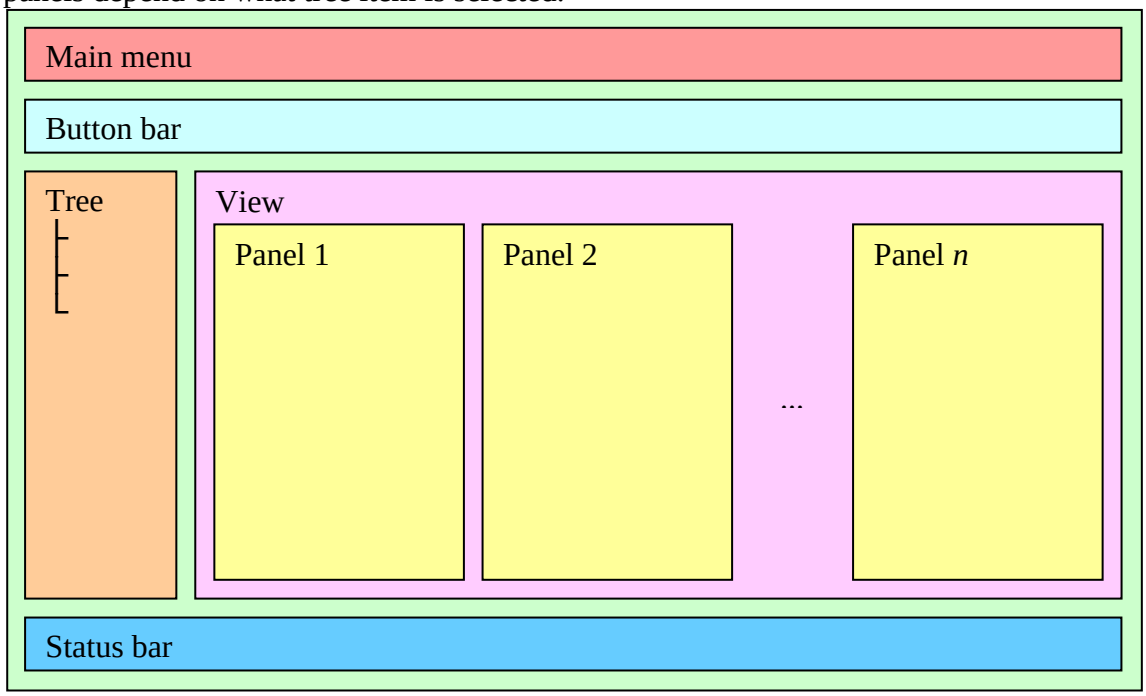
General structure of the user interface is as follows (hierarchy is usually Window = Bars + Tree + View containing various Panels):

- Main window 2.1
  - Main menu 2.2
  - Button bar 2.3
  - Tree 2.4
  - View (always Title panel 2.5.1 and Notes panel 2.5.2 and possibly other panels)
    - **Region view**
      - X-data range panel 2.5.3
      - Analyzer settings panel 2.5.4
      - X/Y adjustments & Quantitative analysis panel 2.5.5
      - Processing panel 2.5.6
      - Table panel 2.5.7
      - Graph panel 2.5.7
    - **MultiView** 4.2.1
    - Photon energy scan view
      - XPD panel 2.5.8
      - Regions panel 2.5.11
      - Scans panel 2.5.12
      - Image panel 2.5.13
    - **Angular scan view**
      - XPD panel 2.5.9
      - Regions panel 2.5.11
      - Scans panel 2.5.12
      - Image panel 2.5.13
    - Sequence scan view
      - XPD panel 2.5.10
      - Regions panel 2.5.11
      - Scans panel 2.5.12
      - Image panel 2.5.13
    - Other views (Title, Notes, Sputtering and/or Annealing, Gas exposure, Deposition)
    - EDAC view
      - ??? panel
      - ??? panel
    - LEED view
      - Load panel 2.5.14
      - Image panel 2.5.15
    - Chart view
      - List 2.5.16
      - MultiView 2.5.17, 4.2.1
  - Status bar
- Monochromator window 3.1.1
- Manipulator window 3.3.1
- Fitting window 4.2.4

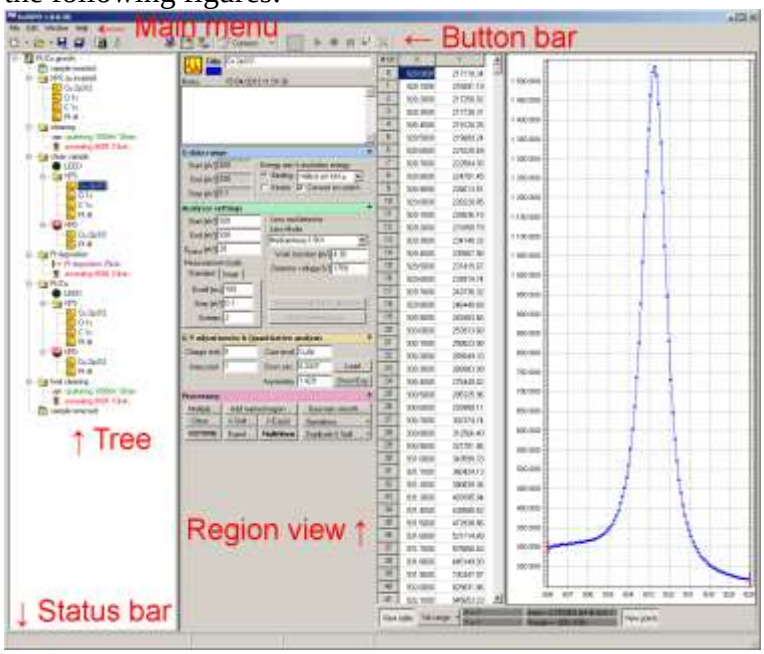
2.1 Main window

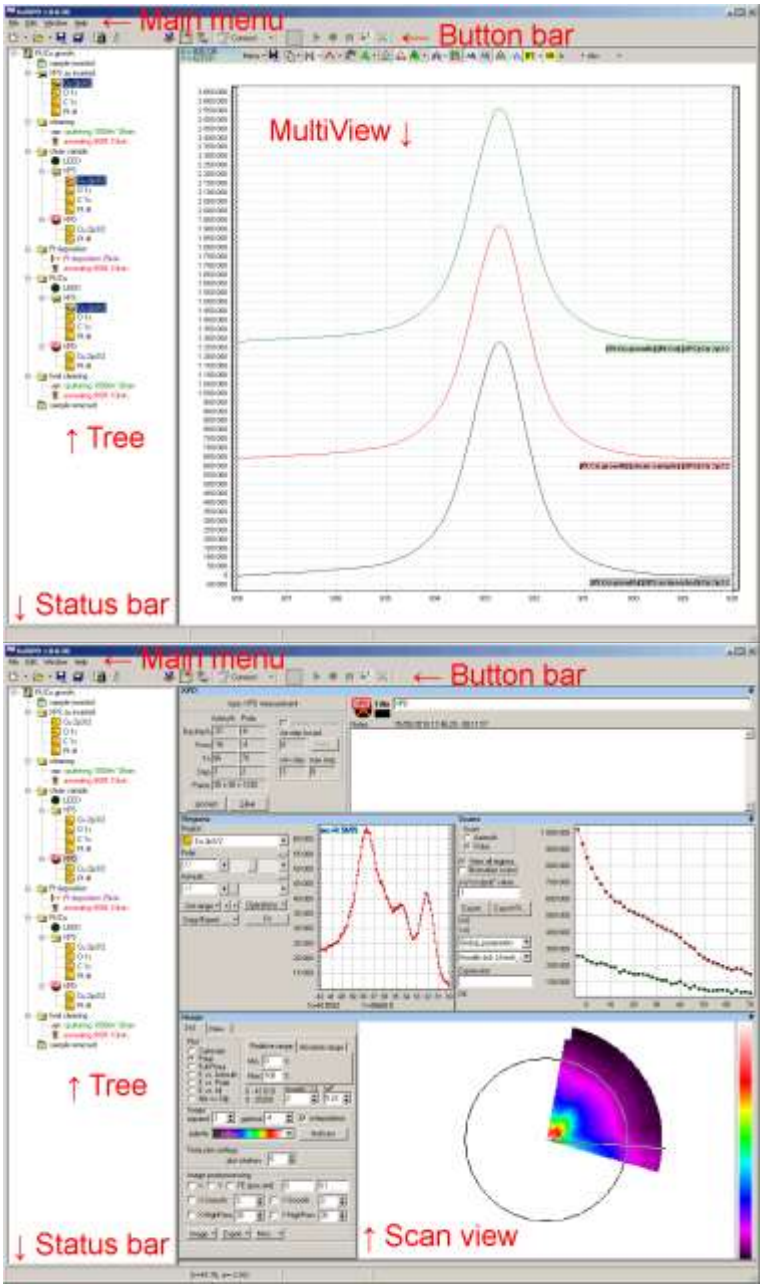
The main window always contains the main menu at the top, the button bar under it and the status bar at the bottom. The area between them is divided vertically in two parts, in

the left part the tree is always displayed while the view on the right side and included panels depend on what tree item is selected.



The most typical Main window views (marked in bold in the list above) are shown in the following figures:





2.2 Main menu

2.2.1 File

- Open: opening files of types listed in 1.5.1. Multiple files can be selected.
- Import: importing VG 2D-detector datafiles, the dialog described in 4.1.5 is shown. More simple files can be imported directly using the Open dialog.
- Save as...: saving the selected item in the tree into a file in one of the formats listed in 1.5.2. The format is based on the type of the item (generally experiments and folders are saved as exp, regions as xps and scans as xpd).
- Save All: saves all root items in the tree.
- Load options
- Load XPD form data: ???
- Copy XPD form data from selected item: ???

- Convert to binding: xml and xy files (that are saved in kinetic energy scale by SpecsLab2) will be automatically switched to binding energy scale upon load to KolXPD.
- Export all fit data...: all fit parameters in the whole exp file will be saved into a single txt file (for the format see Saving fit parameters in 4.2.4).
- Register file extension association: associates cls, exp, pd, xml, xpd, xps and xy files with KolXPD. Such files can be then directly open from Windows Explorer and other file managers.
- Exit: exit KolXPD

2.2.2 Edit

- Cut: cuts selected item(s) into clipboard.
- Copy: copies selected item(s) into clipboard.
- Paste (into): pastes item(s) from the clipboard into the selected item.
- Paste after: pastes item(s) from the clipboard after the selected item.
- Copy path(s): copies the tree paths of the selected item(s) into clipboard.
- After mouse move/copy: insert log into Notes: when the selected item(s) are dragged-and-dropped by mouse somewhere else in the tree information about this movement is logged in the corresponding Notes panel.

2.2.3 Window

- KolXPD: main window (see 2.1).
- Monochromator (if open): control of the beamline monochromator, setting the photon energy (see 3.1.1).
- Manipulator (if open): control of the sample manipulator, setting the azimuth/polar angle of the sample with respect to the electron analyzer (see 3.3.1).
- Fitting (if open): main interface of the curve fitting module (see 4.2.4).

The latter 3 windows can be kept always on top, minimized/restored and closed by these buttons located in their top right corners, respectively: . They can be also moved by dragging their header a resized by dragging their black bottom right corner ⌟.

2.2.4 Help

- About: information about the installed version, license, author contacts, project webpage and possible update if the computer is connected to internet.

2.3 Button bar

 create a new item in the tree of the selected type (see 2.4.1).

 open files of types listed in 1.5.1. Multiple files can be selected. Clicking on the arrow symbol allows choosing from recently opened files.

 save the selected item in the tree into a file in one of the formats listed in 1.5.2. The format is based on the type of the item (generally experiments and folders are saved as exp, regions as xps and scans as xpd).

 save all root items in the tree.

 show/hide colors of all items independently on if they are currently displayed or not.

 blend items of the tree containing only information but no data.

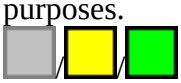
 show/hide Manipulator control window

 show/hide analyzer control bar under the Button bar

 show/hide Monochromator control window



connect/disconnect electron analyser. The arrow on the right side permits to select real Phoibos 150 analyzer or computer simulation for testing purposes.

 analyzer is disconnected/connected in standby mode/currently acquiring.

 start acquisition.

 abort acquisition.

 pause/resume acquisition.

 automatically save the acquired data after each scan in the autosave.xpd (or autosave.exp?) to the user directory (usually C:\ Documents and Settings\[user]\Application Data\kolibrik.net\KolXPD).

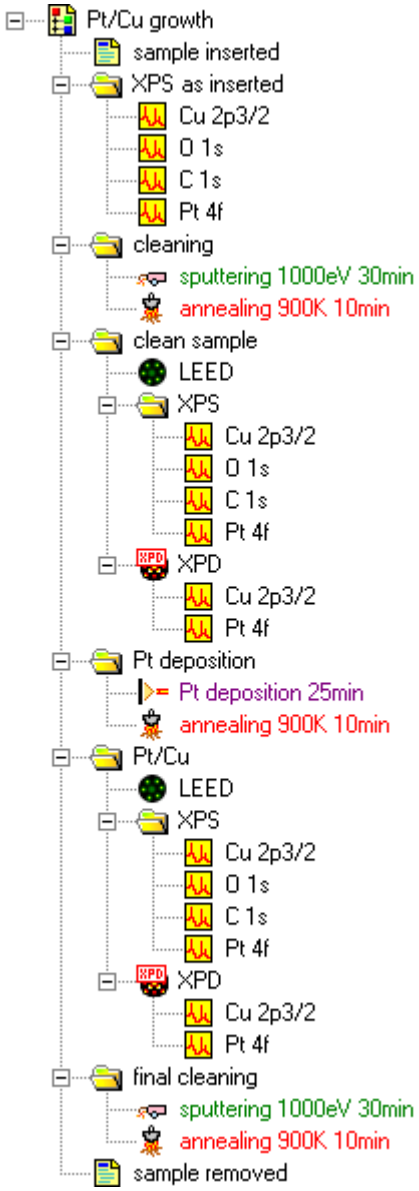
 automatically disconnect the analyzer after finishing the scan (does not work with Simulation).

The analyzer bar shows the status of the analyzer. It is by default shown when the analyzer is connected and hidden when disconnected but this behaviour can be overridden by the  button above. For example when the angle-resolved scan is running it shows the actual energy of the analyzer (cyan), current status of the scan (points acquired/total points, percentage, yellow), current status of the region acquisition (current sweep/total sweeps, percentage, region title, yellow), status (green if OK and red in the case of error) and buttons for controlling the acquisition and display, see 3.1-3.4 for details.



2.4 Tree

The experiment is organized in a tree structure that is always displayed in the left part of the user interface. The root of the tree is the experiment file which can contain the acquired data or information about the course of the experiment organized in folders. Therefore KolXPD can serve also as electronic logbook of the experiment. An example of the tree structure of the experiment is shown here:



All items of the tree have a specific path under which they are saved in exp files. The syntax of the path is
[file]\[folder]\[subfolder]\...\item,
for example the path of the "O 1s" XPS region acquired on the clean sample above would be
[Pt/Cu growth]\[clean sample]\[XPS]\O 1s.
The expressed part is used for labelling corresponding curves in MultiView (see 4.2.1).

2.4.1 Tree items

All possible items of the tree are listed in the following table:

icon	*name*	*purpose*	*panels (see 2.5)*
General items			
	Experiment	root of the experiment	Title, Notes
	Folder/Subfolder	grouping of similar items	Title, Notes
Items containing photoemission data			
	Region	one photoemission region (a set of energy-intensity pairs)	Title, Notes, X-data range, Analyzer settings, X/Y adjustments & Quantitative analysis,

			Processing, Table, Graph
	Photon energy scan	set of equal regions acquired with different photon energies (e.g. resonant photoemission, X-ray absorption, energy-resolved photoelectron diffraction	Title, Notes, XPD, Regions, Scans, Image
	Angular scan	set of equal regions acquired with different azimuth/polar angles of the sample manipulator	Title, Notes, XPD, Regions, Scans, Image
	Sequence scan	time sequence of the set of equal regions	Title, Notes, XPD, Regions, Scans, Image
Other items			
	Sputtering	information about ion sputtering of the sample (e.g. ion energy, time, current, pressure)	Title, Notes
	Annealing	information about annealing of the sample (e.g. temperature, time, pressure)	Title, Notes
	Sputtering + Annealing	information about ion sputtering of the sample at elevated temperature	Title, Notes
	Gas exposure	information the gas exposure (e.g. type of gas, pressure, time, sample temperature)	Title, Notes
	Deposition	deposition of something on the sample (e.g. type of material, evaporator parameters, pressure, time)	Title, Notes
	LEED	information about LEED acquired, acquired images can be included (no idea if/how this function works)	Title, Notes, Load, Image
	EDAC cluster	cluster file for EDAC XPD pattern calculations	Title, Notes, ???
	EDAC result	result of EDAC calculated XPD pattern. 2D angle data, each angle point contains only a number - calculated intensity	Title, Notes, ???
	Title	general title	Title, Notes
	Notes	general notes	Title, Notes
	Chart	set of curves to be displayed in MultiView (see 4.2.1)	Title, Notes, List, MultiView

2.4.2 Tree operations

A number of operations can be performed on each item:

- Selection (works like standard windows tree control):
  - Single selection by single click, browsing by ↑/↓.
  - Expand/collapse of folder by left double-click , left click on +/– sign, keypad +/– or →/←.
  - Multiple selection by Ctrl/Shift + left click or Shift-↑/↓. Multiple selection using Shift is adjusted in order to contain items of single type (you can click on some region and that Shift + left click on a region in different folder, then all regions between will be selected but not folders and other items) so the selection is consecutive. Multiple selection using Ctrl serves for non-consecutive items.
  - If you have multiple selection and left click on some selected item, other items will not be unselected.

- Arrangement:
  - You can move items by drag-and-drop with mouse. Only one item can be dragged.
  - If you hold Shift or Ctrl during drag-and-drop, item will be copied.
  - You can move (reorder) selected items within a folder by pressing Alt-↑/↓. This works for multiple selection.
  - You can cut/copy/paste (multiple) selection using Ctrl-C and Ctrl-V, the main or the context menu. (Tip: Items are copied into clipboard as text in same format that is used for saving to files. You can alter text in a notepad before paste back or used its data in other software.)
- Other:
  - You can double click on the region title in order to display it in MultiView (see 4.2.1).
  - You can change the Title of any item by second left click on it.
  - The context menu is available by right click on the item or selection.
  - One item at the time can be highlighted in yellow by pressing Space when selected (or in the context menu, see 2.4.3), such marked region will be used for operations of addition to/subtraction from other region as described in 4.2.3.

2.4.3 Tree context menu

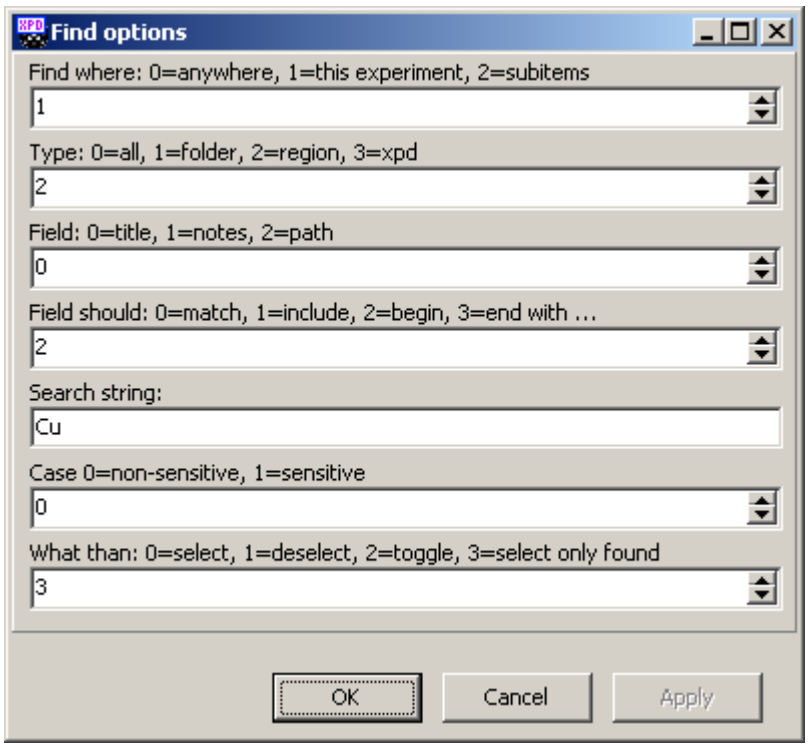
In the tree the context menu displayed by right click on any selected item(s) permits to perform the following operations (if available):

- Save as...: saving the selected item in the tree into a file in one of the formats listed in 1.5.2. The format is based on the type of the item (generally experiments and folders are saved as exp, regions as xps and scans as xpd).
- Update/Append: adds to the current tree item all new or updated items from the selected file(s). It can be useful for merging more experiment files together or in the case that the original file has been modified in the meantime (e.g. new groups added by SpecsLab2 into the file). Updated/appended items are then labelled by sign.
- New: creates a new item in the tree of the selected type (see 2.4.1).
- Change item: always blended???
- Delete: deletes the item(s) from the tree (no files are physically deleted from the file storage).
- Convert to prm-resolved experiment: KolXPD can automatically operate e.g. a motor-controlled sample manipulator and acquire photoelectron data at each emission angle. In the case you have a set of 2D data measured at different emission angles set manually (or any other parameter-dependent set of 2D spectra) you can convert them using this function into a 3/4D dataset and then handle them like if they were measured automatically by KolXPD. For details see 4.1.6.
- Set to all items: permits to perform several operations at once on all selected items, most of them only on regions (Title and Notes also in other cases). The possibilities are:
  - Title: sets the title.
  - Level: sets the photoelectron level of the region(s) (see 2.5.5).

- Cross-section: sets the photoionization cross section of the region(s) (see 2.5.5).
- Asymmetry: sets the photoelectron level of the region(s) (see 2.5.5).
- Charge shift: sets the charge shift value of the region(s) (see 2.5.5).
- Apply shift and set it to 0: permanently shifts the spectra by the value in the Charge shift field (i.e. modifies the X-axis) and then sets this value to 0 in order to avoid another shift if the operation was repeated.
- Area coef. (or mc): sets the area coefficient (that may e.g. represent the photon flux) of the region(s) (see 2.5.5). If the region(s) title contains the string "mc [*value*]" write "mc" in this field and KolXPD will use this [*value*] (see 4.1.2).
- Delete mc record from region title: if KolXPD uses the "mc [*value*]" it will delete it from the region(s) title afterwards.
- Multiply spectra by area coef. and set it to 1: multiplies the intensity (Y-axis) by the value in the Area coef. field and sets it to 1 afterwards in order to avoid another scaling if the operation was repeated. This operation may represent e.g. the normalization of the spectra intensity to the incident photon flux (see 4.1.2).
- Excitation energy: sets the photon energy of the region(s) to the chosen value (see 2.5.4).
- Axis: switches the X-axis of the region(s) to binding or kinetic energy scale based on the Excitation energy set (see 2.5.4).
- Permanently correct to analyzer transmission: divides the intensity (modifies the Y-axis) by the transmission function of the electron analyzer. At the moment the shape of the transmission function shape is set as ideal in the "constant pass energy" acquisition mode, i.e. $(\text{kinetic energy})^{-1}$.
- Color: sets the color of all selected spectra in MultiView (see 4.2.1).
- Copy group color to all regions (direct children): sets the color of all subitems of the selected folder to the one defined for it.
- Notes: sets the notes of the selected item(s). All previous notes (if present) will be deleted.
- Reload cross-sections from database: loads the photoionization cross section values from the database based on the region(s) level field, see 2.5.5.

- Enumerate: adds/removes numbers from the item title. Several options are available:
  - All (direct children): enumerates all direct subitems. If any numbering is already present it will be replaced. You can select the number to start with.
  - Groups/folders (direct children): enumerates only direct subitems that may contain data (folders, scans, regions charts); items containing only information are skipped. If any numbering is already present it will be replaced. You can select the number to start with.
  - All siblings from here down: enumerates all items in the same folder starting from the selected item down. If any numbering is

already present it will be replaced. You can select the number to start with.
    - Sibling groups/folders from here down: enumerates only items that may contain data (folders, scans, regions charts) in the same folder in from the selected item down; items containing only information are skipped. If any numbering is already present it will be replaced. You can select the number to start with.
    - Remove from direct children: removes numbering from all direct subitems if present.
    - Remove from here down: removes numbering from all items in the same folder from the selected item down if present.
- Mark item: marks the selected region that contains data to be added to/subtracted from the data in other region, see 4.2.3 for details.
- Cut: cuts selected item(s) into clipboard.
- Copy: copies selected item(s) into clipboard.
- Paste (into): pastes item(s) from the clipboard into the selected item.
- Paste after: pastes item(s) from the clipboard after the selected item.
- Auto-colorize children: changes the color of curves for MultiView (see 4.2.1) of all regions in the selected folder in order that they can be easily distinguished.
- Expand/Collapse: expand or collapse all subitems of the selected item(s).
- Export tree: export the tree structure as text.
- Select: selection of items based on the following criteria:
    - All items with same name: all items that have the same title as the selected item.
    - Visible items with same name: visible items that have the same title as the selected item (i.e. those that are not inside collapsed folders).
    - All in current experiment: all items that have the same title as the selected item and belong to the same experiment file.
    - Visible in current experiment: visible items that have the same title as the selected item (i.e. those that are not inside collapsed folders) and belong to the same experiment file.
    - By path...: the items of the specified path (for path see 2.4).
- Deselect: excluding items from the already-made selection based on the same criteria as selection, i.e.:
    - All items with same name: all items that have the same title as the selected item.
    - Visible items with same name: visible items that have the same title as the selected item (i.e. those that are not inside collapsed folders).
    - All in current experiment: all items that have the same title as the selected item and belong to the same experiment file.
    - Visible in current experiment: visible items that have the same title as the selected item (i.e. those that are not inside collapsed folders) and belong to the same experiment file.
- Find items: more general lookup for items that comply with the specified criteria: In the following example



will be selected all regions in the selected experiment file of which title begins with the case-non-sensitive string Cu (i.e. Cu, cu, CU, cU).

2.5 Panels

Some panels can be shown or hidden by clicking on the ⬍ symbol in the top right corner.
Follows the list of panels:

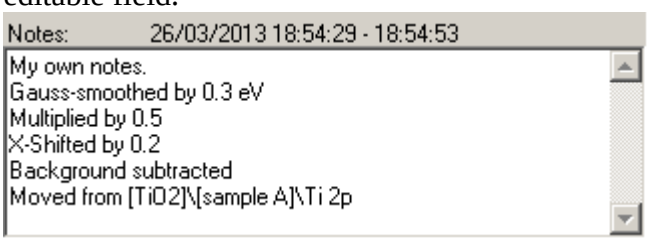
2.5.1 Title panel

The title panel displays the type (for icons see 2.4.1), title and color of the item. If the type is Experiment file it also contains the path and filename on the computer storage. The box with the title name enables to modify the title. The color bar under the title indicates the color of the region in MultiView (see 4.2.1). The color may be changed by clicking on the color bar.



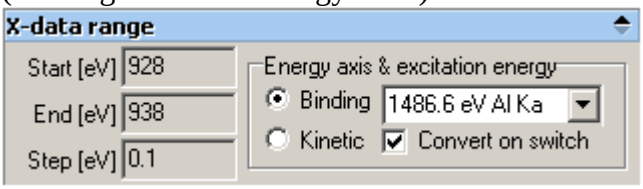
2.5.2 Notes panel

The notes panel can be edited. All notes will be stored once the file is saved. Most of the processes performed on the region spectrum will be automatically logged in the Notes panel. If the data were acquired using KolXPD the date and time of acquisition (begin-end) is displayed above the editable field.



2.5.3 X-data range

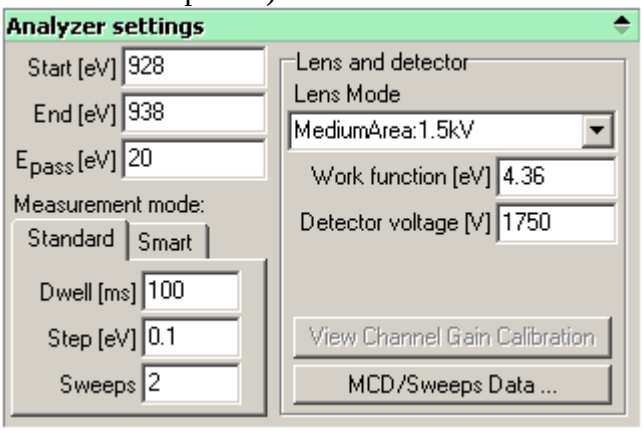
This panel contains the information about the energy range (X-axis) of the region if any data present (Start, End, Step) and the type of this axis (Binding or Kinetic energy scale).



Switching between Binding and Kinetic buttons with unchecked Convert on switch button will merely reverse the X-axis of the spectrum. In order to transform the kinetic energy scale to the binding energy scale and vice versa, the Convert on switch button must be checked and appropriate excitation energy must be entered in the edit box. The spin button allows choosing one of two typical X-ray sources (Al Ka with the excitation energy of 1486.6 eV and Mg Ka with the excitation energy of 1253.6 eV), previously entered custom values or Monochromator (that will read the actual value from the beamline monochromator if present). For details about the acquisition see 3.1.

2.5.4 Analyzer settings panel

This panel contains the analyzer parameters of the region to be acquired (see 3.1-3.3) or already acquired (see 4.1.2) if available: start, end, pass energy, lens mode, work function of the analyzer and the voltage on the multiplier, the measurement mode (standard/smart) and further parameters depending on this mode (dwell time, energy step and number of sweeps/dwell time and number of snapshots). For details about these modes see 3.1.

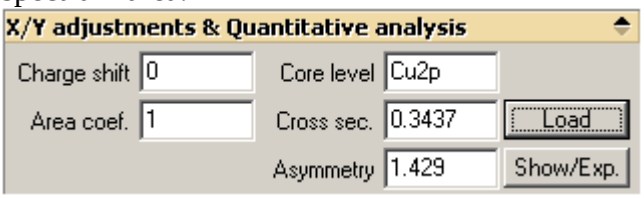


Two other buttons are available: View Channel Gain Calibration for the Smart measurement mode (see 3.1) and MCD/Sweeps Data... for browsing the complete information included in SpecsLab2 xml files where different channel and sweep data are saved separately. This allows excluding the unwanted parts disturbing the acquired spectrum, e.g. if one multiplier was generating strong noise or if during some sweeps the photon source was unstable. Another example may be to compare the spectrum from the first and the last sweep to check the stability of fast-degrading samples under X-ray illumination. For details see 4.1.2.

2.5.5 X/Y adjustments & Quantitative analysis panel

The panel contains the parameters used in MultiView (see 4.2.1) for data displaying and fast quantitative analysis, the raw data remain unaffected.

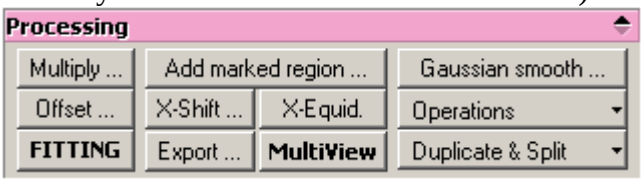
The Charge shift will shift the energy scale (X-axis) by the entered value on pressing the Charge shift button in MultiView (see 4.2.1) e.g. if all spectra are shifted due to surface charging of the measured sample. The parameter Area coef. will take effect in MultiView on pressing Normalize button with checked Multiply by parameter region.area menu item, the intensity (Y-axis) will be multiplied by the Area coef. value. The parameter may be used e.g. to reflect the primary photon flux and affects the calculation of the spectrum area.



Parameter Cross sec. represents atomically calculated photoionization cross section for the corresponding Core level and photon energy (up to 1500 eV) if found in the built-in database [source: http://ulisse.elettra.trieste.it/services/elements/WebElements.html]. The cross section values are used for fast quantitative analysis in MultiView (see 4.2.1). The Asymmetry value comes from the same source but it is currently not used for any calculation (the angular correction factor is ignored). Both values can be modified or loaded from the database by clicking the Load button. The button Show/Exp. permits to show their photon-energy dependence and to export it using the universal Export window (see 4.2.5). We remark that this approach to XPS quantitative analysis is very simplified, supposes homogeneous samples with atomically flat surface, ideal shape of the transmission function of the analyzer $(\text{kinetic energy})^{-1}$, and should be therefore considered as rough estimation of the sample composition. For details see 4.2.1.

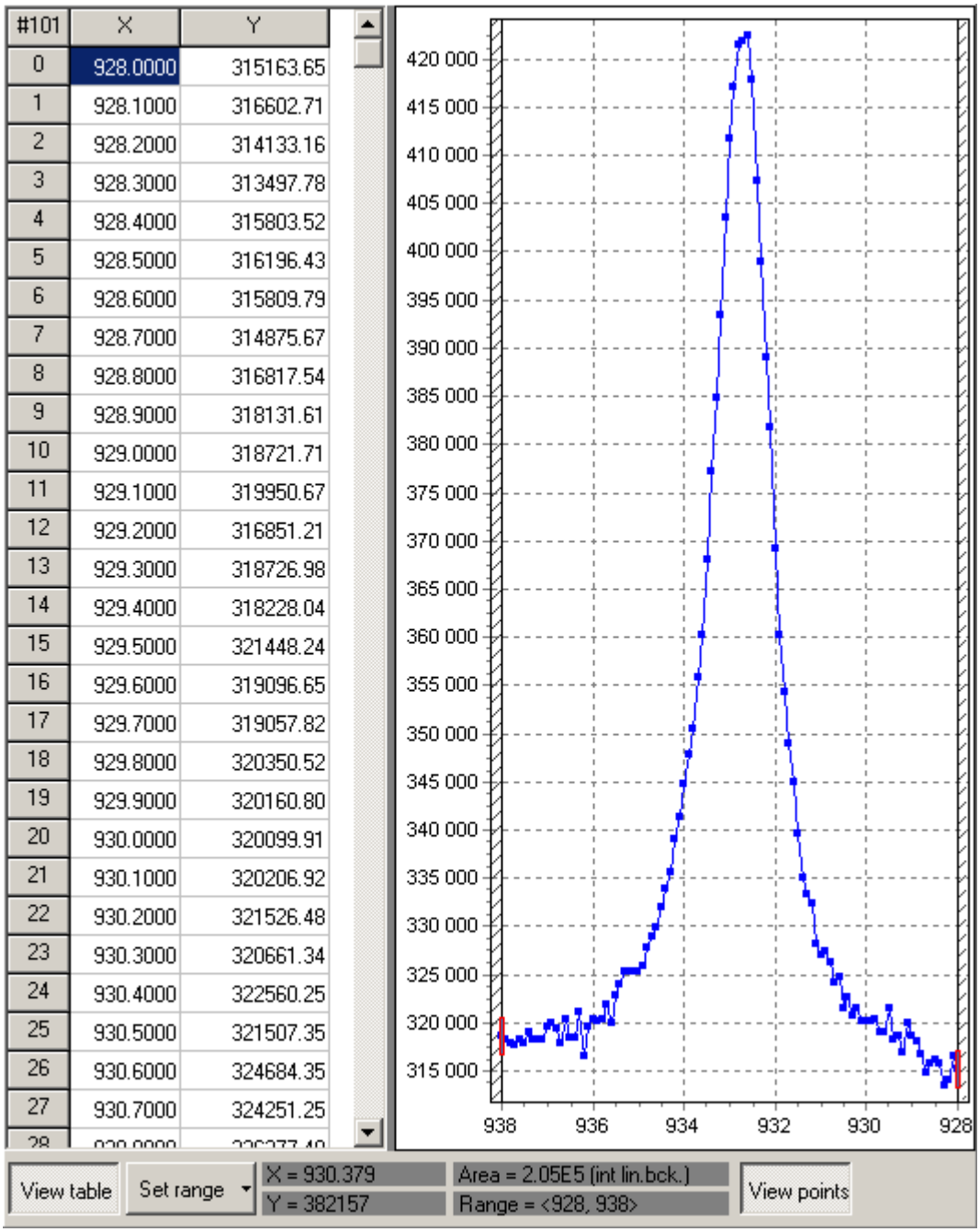
2.5.6 Processing panel

This panel permits to perform modifications of the raw data by several operations: multiply and offset the intensity scale (Y-axis), add or subtract the data from another region (marked by yellow in the tree (see 2.4.2), smooth the data using a Gaussian filter, shift the energy scale (X-axis) and make it equidistant of chosen step, duplicate the region or divide it in more new regions of the chosen energy range, display the data in MultiView (see 4.2.1), fit them (4.2.4), export them (4.2.5) and perform other operations (permanently subtract the secondary electron background or correct the intensity scale when the detector is not linear).



2.5.7 Table and Graph panels

The table containing the data of the selected region can be displayed by clicking on the View table button in the bottom part. The values in the table can be modified by double-clicking on the desired cell, e.g. for removing spikes. The total number of points is written after the # in the top left corner.

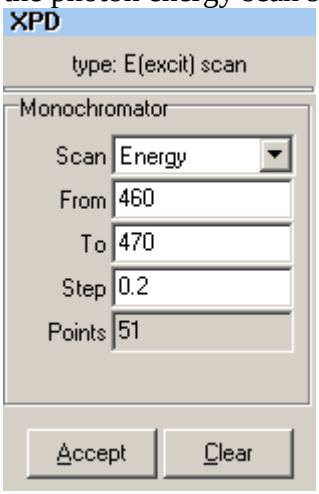


In the right part the graphical representation of the region data is displayed, the fields in the lower part show the actual X and Y position of the mouse pointer, total spectrum if linear background was subtracted and the selected data range for further data processing. In the figure the range for processing (hatched lines) corresponds to the full range where the data were physically acquired (red vertical bars). Using the Set range button the range for processing can be modified according to the zoomed area or back to full range or the borders can be set from the keyboard. Another possibility is to set the range for processing by mouse as described in 2.7.

2.5.8 XPD (for photon energy scans) panel

In allows setting of the parameters of the monochromator during the scan. The typical choice is to set the tuned photon energy lower and upper limit and step. In the Points field a total number of points of the photon energy scan is shown. After clicking on Accept the editable fields are locked, if the values do not comply with the limits set in the configuration file (see 1.4.5)

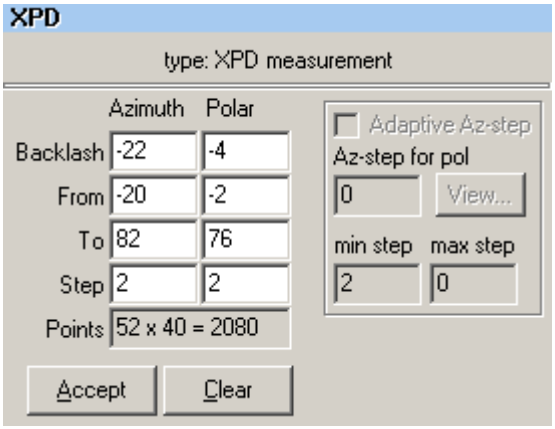
they will be automatically adjusted. For details concerning the acquisition of the photon energy scan see 3.2.



For unlocking the fields click on the Clear button. Use the same button also for clearing the scan from previously acquired data.
Other possibilities of the monochromator scan is to move only one axis (PM - plain mirror, PG - plain grating) which might be sufficient for narrow energy scan, or to scan the Cff parameter of the monochromator (mainly for calibrating purposes).

2.5.9 XPD panel

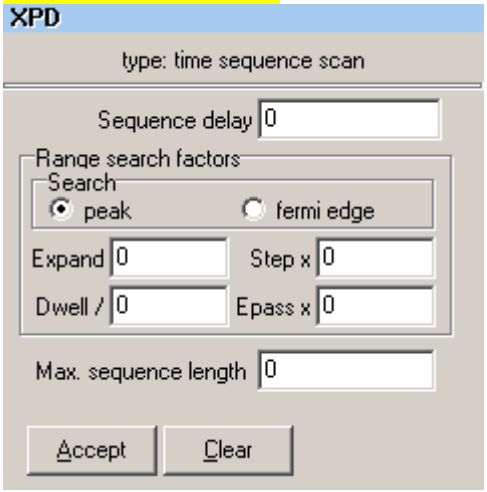
It allows setting of the parameters of the sample manipulator (polar and azimuthal angle) during the scan. The polar angle change is in the inner loop in order not to move the azimuth angle too often (outer loop) - maybe in Prague it's opposite!. The editable fields contain the lower and upper limits of each axis, corresponding angular steps and absolute backlashes (i.e. the angles set before each scan in order not to change the direction during the scan; in the example in the figure both backlashes are 2 degrees below the starting value). To scan only one axis set the other one's Backlash = From = To.



In the Points field the total number of points of the angular scan is shown. After clicking on Accept the editable fields are locked, if the values do not comply with the limits set in the configuration file (see 1.4.5) they will be automatically adjusted. For details concerning the acquisition of the angular scan see 3.3.
For unlocking the fields click on the Clear button. Use the same button also for clearing the scan from previously acquired data.
no idea how Adaptive Az-step work, do they use it in Prague???

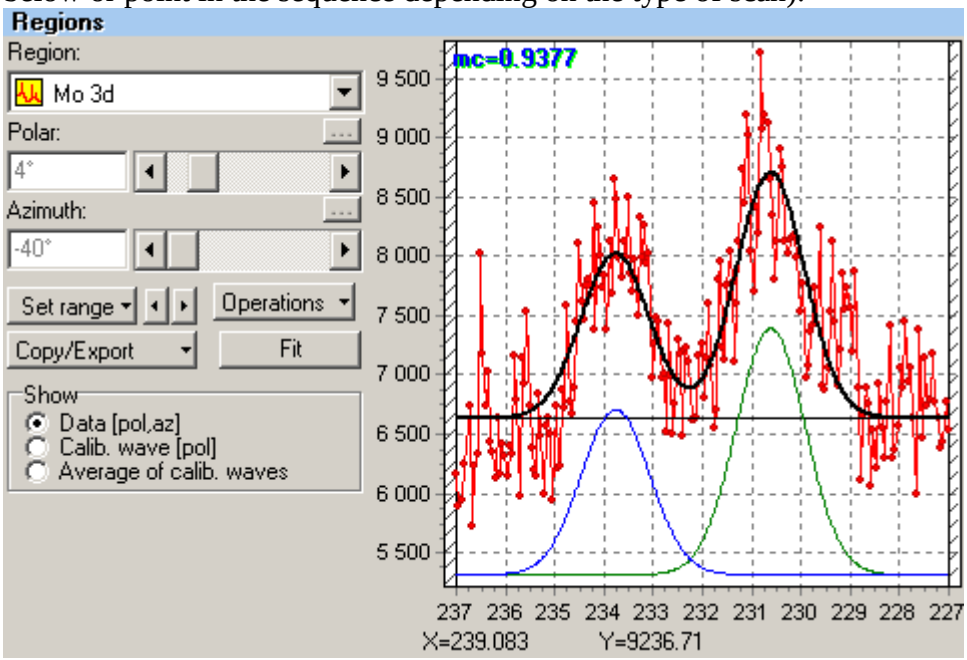
2.5.10 XPD (for sequence scans)

no idea how it works.



2.5.11 Regions panel

This panel allows browsing and processing the spectra acquired during photon energy, XPD and sequence scans. The user can choose which region to view (if more than one are or were acquired), current position in the whole scan (photon energy, azimuth/polar angle shown in the example below or point in the sequence depending on the type of scan).

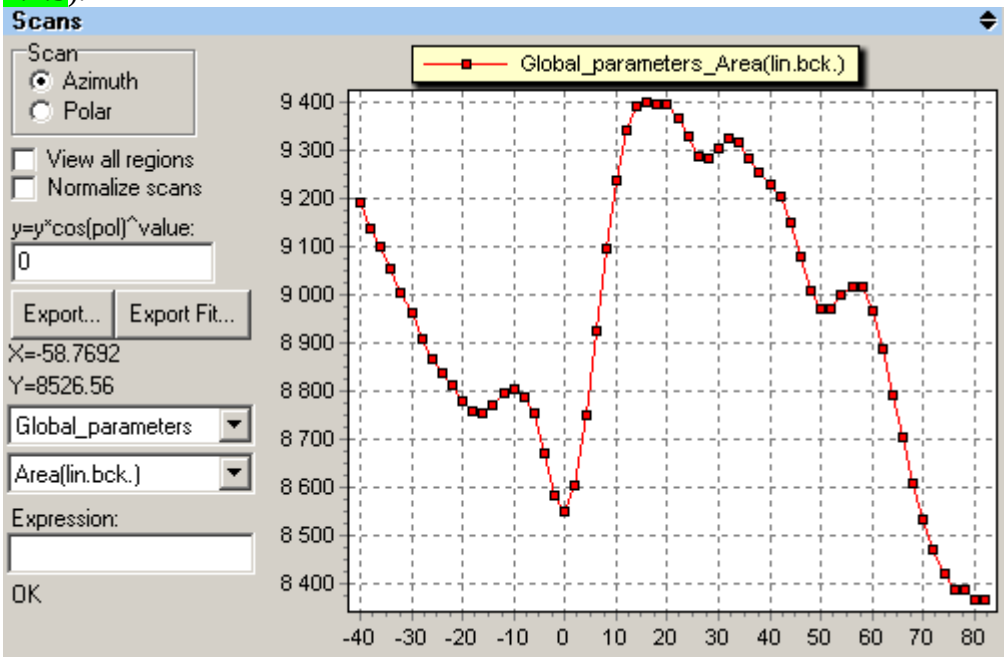


The range of the graph can be set using the corresponding button or by mouse (see 2.7) and then the data can be modified by several operations, fitted (see 4.2.4) and exported (4.2.5). For details see 4.3-4.5.

2.5.12 Scans panel

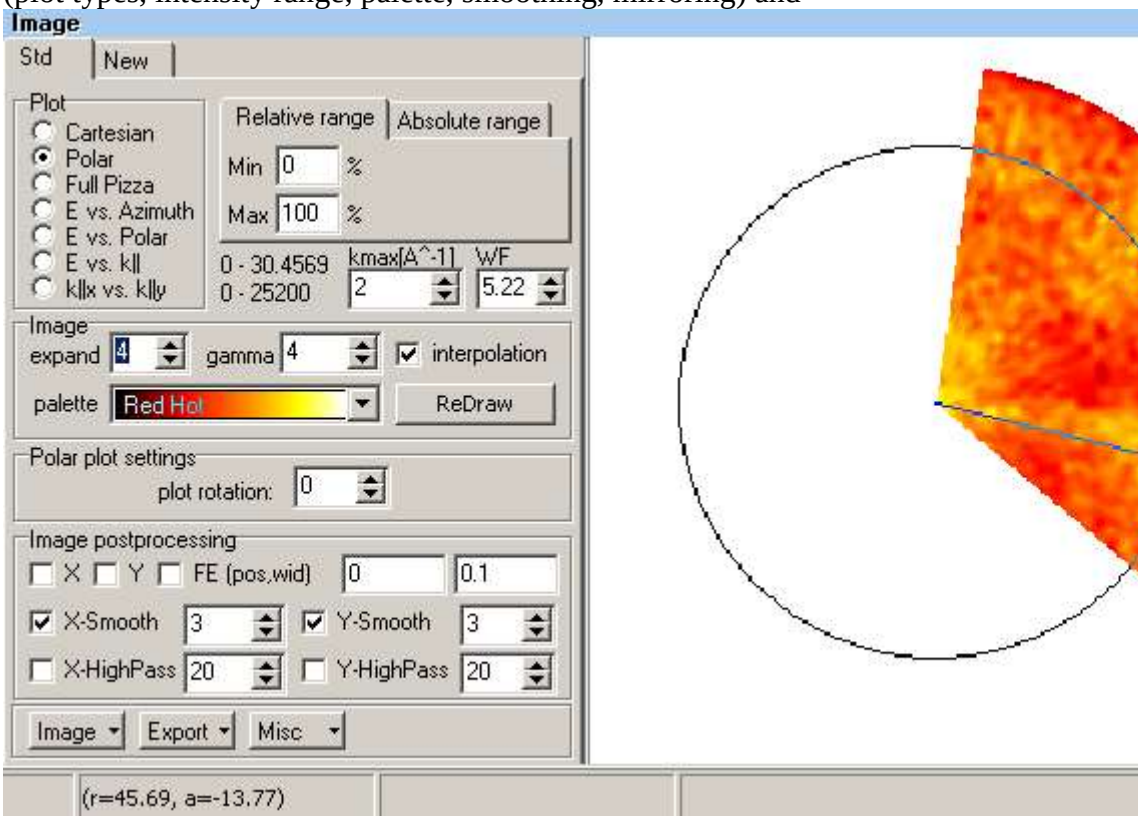
This panel shows the evolution of the selected parameter (e.g. peak intensity) with the variable of the scan, i.e. photon energy, azimuth/polar angle or the point of the sequence. The parameter resulting from more regions acquired at the same time can be displayed and normalized simultaneously (if present). The displayed parameter can come from the raw data of from their fit and the curve can be again exported as usually (see

4.2.5).



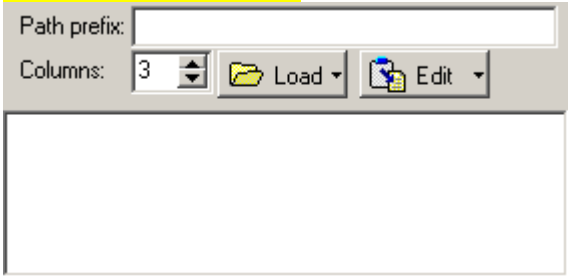
2.5.13 Image panel

It represents the graphical output of the Scans panel, the following example shows the result of the XPS scan. Again many viewing options are available (plot types, intensity range, palette, smoothing, mirroring) and



2.5.14 Load (LEED files) panel

no idea if/how it works

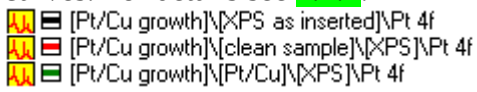


2.5.15 Image (for LEED) panel

no idea if/how it works

2.5.16 MultiView list panel

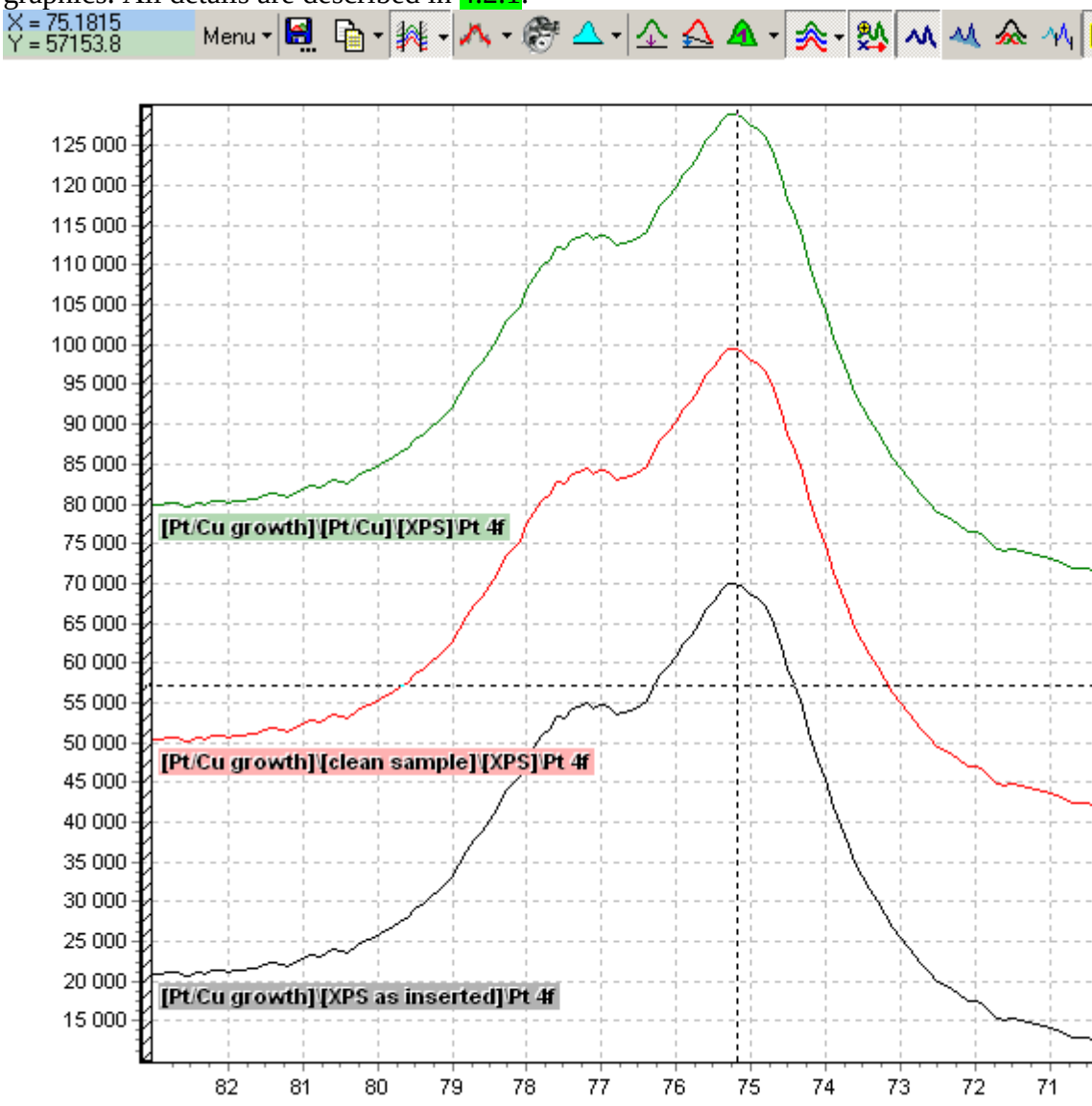
It contains the list of curves displayed in the Chart (always in MultiView) including the corresponding colors and paths (for path see 2.4). The curves in the list can be shown/hidden by pressing Space, double left click or in the context menu under the right click. The same menu permits to edit the list of curves (add/modify/delete their paths) and to select the region(s) of all listed curves. For details see 4.2.1.



2.5.17 MultiView graph panel

It is the main output window of KolXPD. It is displayed always when more than one region is selected in the tree (for displaying only one region you must double-click on it or select MultiView in the Processing panel described above). Permits to construct graphs of one or multiple curve(s) with a number of viewing options, change the range, subtract the background, normalize the spectra, fit all curves by similar analytic curves, perform simplified quantitative XPS analysis and export the all spectra and/or fitted curves ordered as displayed, either as table with values or as

graphics. All details are described in 4.2.1.



2.6 General context menu

General context menu displayed by right click on any editable field contains six simple operations:

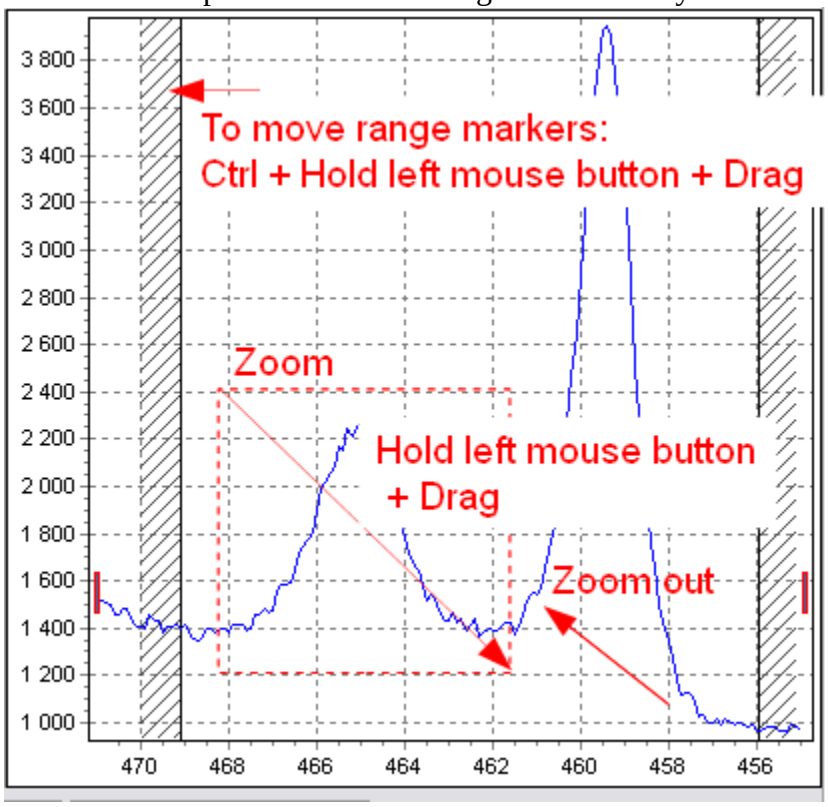
- Undo
- Cut
- Copy
- Paste
- Delete
- Select All

2.7 Graph operations

As seen above many panels contain graphs. Here we list the graph control options:

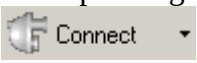
- Zoom (selecting graph area for viewing):
  - Zoom - zoom a region of graph by click and drag a rectangle by mouse. You must start in upper-left corner and go down and right.
  - Unzoom - zoom to fit all displayed data by dragging in opposite direction - anywhere in graph from down-right to up-left.
  - Pan - if graph is zoomed you can catch it by right mouse button and move.

- Range (used to define a part of a wave for subsequent processing, e.g. area and background calculation, fitting, export, etc.):
  - If displayed wave(s) has defined range and can be modified, range borders are displayed by black vertical lines with hatching.
  - You can move with a border by dragging and holding Ctrl key.
  - If you hold Ctrl and Shift it will move both borders simultaneously.
  - Graph can have a Set range button nearby for other range manipulations.



3 Data acquisition

KolXPD is currently designed to acquire photoemission data using Specs Phoibos 150 hemispherical electron analyzer with two types of detectors, MCD9 (9 discrete electron multipliers) or 1D-DLD (one-dimensional delay-line detector providing 100 channels). The setting of the analyzer parameters is very similar to that one used in SpecsLab2. Before the acquisition the analyzer (disconnected in SpecsLab2) must be connected to KolXPD using the corresponding button in the Button bar (see 2.3) and after the acquisition disconnected.



In addition, KolXPD can automatically acquire one or more regions with different photon energy (synchrotron radiation monochromator) or sample position (manipulator) setting, or perform sequence scans in selected time intervals. For the photon energy setting KolXPD communicates with the Kleopatra software at the Materials Science beamline in Trieste that sets the photon energy of the monochromator and provides information about the actual photon flux on the sample, the so called *mesh current*, *mc*. For changing the polar and azimuth angle of the sample with respect to the axis of the analyzer entrance optics KolXPD communicates with the MotorControl software (in Trieste) or xxx (in Prague) that control the stepping motors of the sample manipulator. Both communication channels must be properly configured as described in 1.4.5 and corresponding programs must be running.

3.1 Region acquisition (2D data: cps – KE/BE)

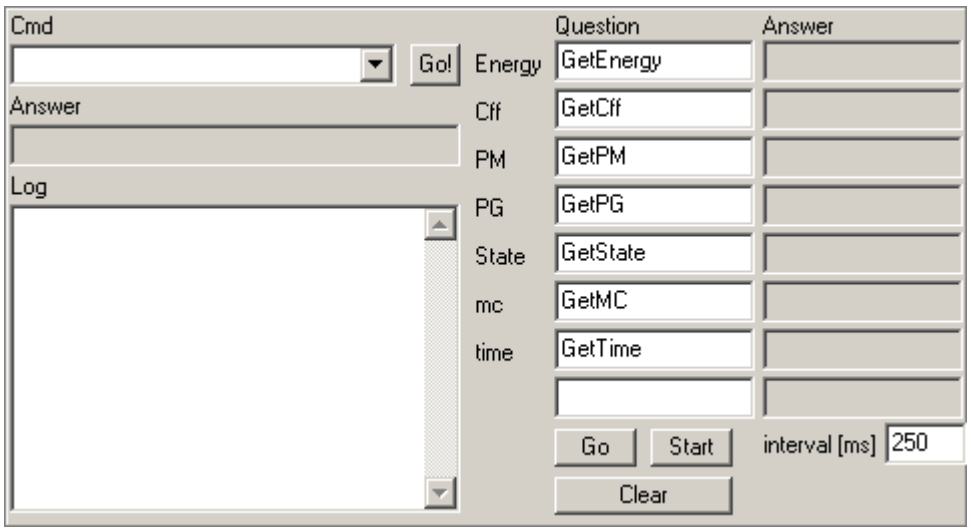
3.1.1 Monochromator window

At the Materials Science Beamline in Trieste KolXPD can automatically set the photon energy by moving the monochromator in the available range. The communication channel must be properly configured as described in 1.4.5.

The photon energy can be set for each region in the X-data range panel (see 2.5.3). In order to see the current status of the monochromator and the progress of tuning click on the  button in the Button bar (see 2.3). The Monochromator window will open:



It shows the current position and status of the monochromator (which can be refreshed by clicking on ) and permits to send three basic commands (setting energy, plain mirror PM or plain grating PG positions to the desired values and clicking the Go button). The button Stop waiting is to be used when KolXPD is blocked by waiting for the response of the monochromator when the communication channel is interrupted. The Log button shows the log of the communication and Cons opens/closes some advanced options:



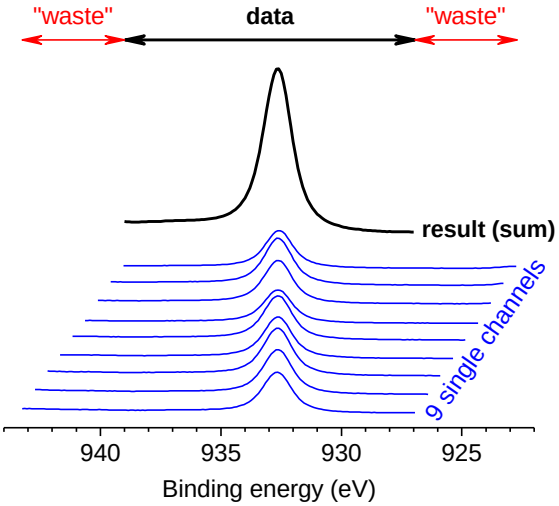
Here, mostly for testing purposes, the user can send more generic commands to the monochromator, usually in the form Get[parameter] and Set[parameter] *value*. On the right side these several Get questions can be asked one (Go button) or repeatedly in the selected interval (Start button).

3.1.2 Standard measurement mode

The acquisition in the standard measurement mode in KolXPD is equivalent to the same action in SpecsLab2 in the FixedAnalyzerTransmission (FAT) mode where the energy resolution is constant. In this mode the entrance optics of the analyzer slows down all the electrons to a constant energy (called *pass energy*, Epass) before they enter the energy filter consisted of two concentric hemispheres and —if they pass— reach the detector. Higher pass energies provide higher transmission (i.e. higher signal-to-noise ratio) but worse energy resolution (being approximately 0.03*Epass).

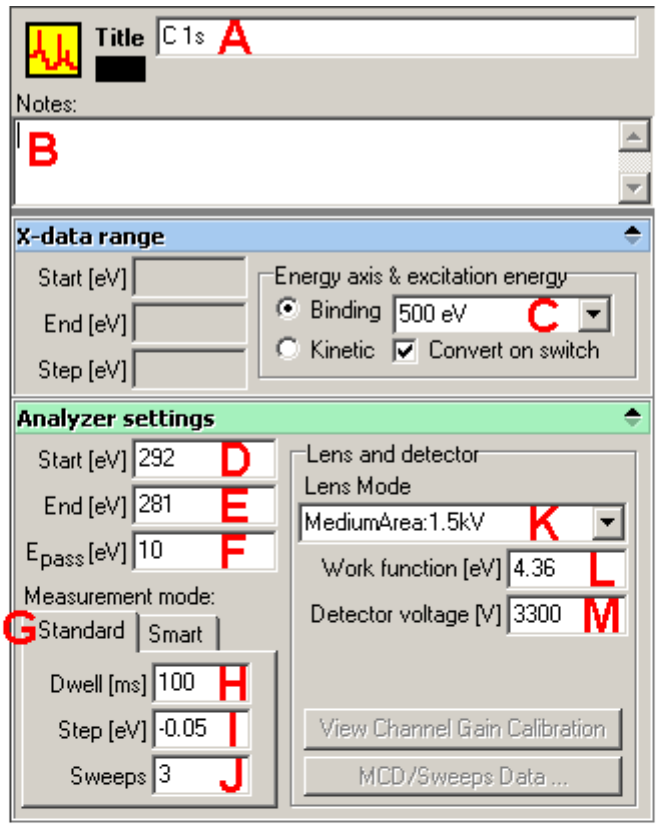
In order to increase the signal modern analyzers are equipped with the so called multichannel detection. For example MCD9 detector of the Specs Phoibos analyzer in Prague has 9 separated electron multipliers distributed over the length of approximately 7 cm after the exit from the hemispheres which can theoretically increase the signal by a factor of 9. However, the spatial distribution of the multipliers results in the fact that each multiplier detects electrons of slightly different energies; the absolute energy spread among all multipliers depends linearly on Epass. It is the task of the acquisition software to align the kinetic energy scale before summing the signals from the multipliers. The calibration procedure is described in the Phoibos and SpecsLab2 manuals and KolXPD should be configured to use the correct dispersion factors as described in 1.4.5.

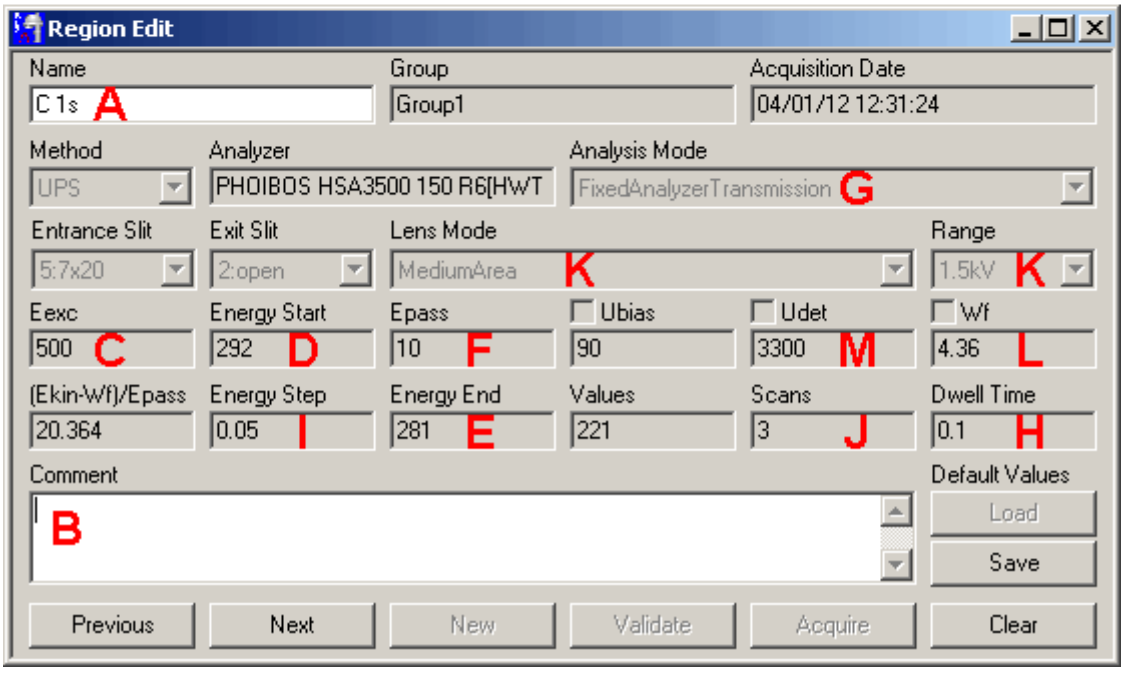
An example of the spectrum acquired in the Standard measurement mode using the MCD9 detector is in the following figure:



As in the selected energy range the data from all 9 multipliers must be available the real acquisition range is extended by the software by 20% of Epass on each side. It means that the real acquisition in the Standard measurement mode will be somehow longer that theoretically needed, in the presented example (12 eV desired energy range, 20 eV Epass) the "wasted" time is 0.4*20/12 is 67%, i.e. in the case of energy step 0.1 eV, dwell time 100 ms and 5 sweeps the acquisition takes 100 s instead of 60 s. Of course the relative "waste" is lower at lower pass energies and broader energy ranges. The figure above also shows that the intensity from various channels can be different (due to different alignment, spatially-dependent transmissions, multiplier ageing...) but in this mode it is not a problem as all data are summed together. The only problem would be if the spectrum shape differed (e.g. some channels producing noise etc.), in such case the faulty data can be omitted during processing (see 4.1.2???).

After setting correctly the acquisition parameters in the X-data range and Analyzer settings panels you can start/abort/pause the acquisition by pressing  buttons and observe the progress in the Button bar (see 2.3). All acquisition parameters in KolXPD have their direct equivalents in SpecsLab2, as can be seen in the following figure:



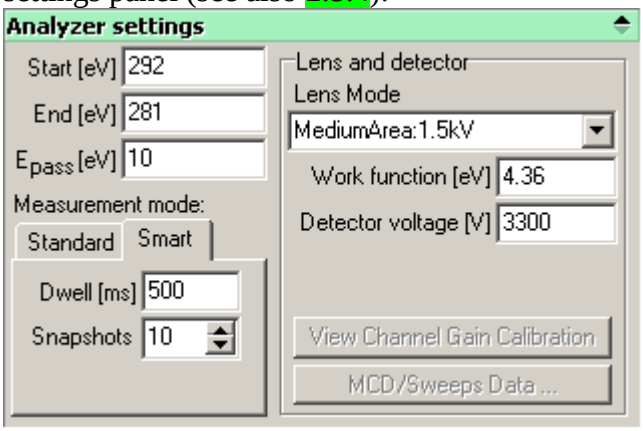


The only practical difference from SpecsLab2 is that the number of sweeps cannot be changed while the acquisition is in progress. (I have a feeling that it WAS possible so maybe it only does not work when Simulation instead of Phoibos analyzer is used. I will test it during next beamtime)

3.1.3 Smart measurement mode

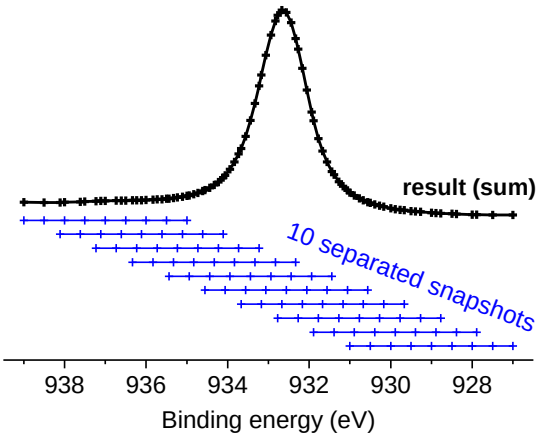
The Smart measurement mode is similar to the Snapshot FAT (SFAT) mode in SpecsLab2 with several differences. With respect to the Standard measurement mode one has to set only dwell time of each snapshot and the

number of snapshots as shown in the following figure of the Analyzer settings panel (see also 2.5.4):



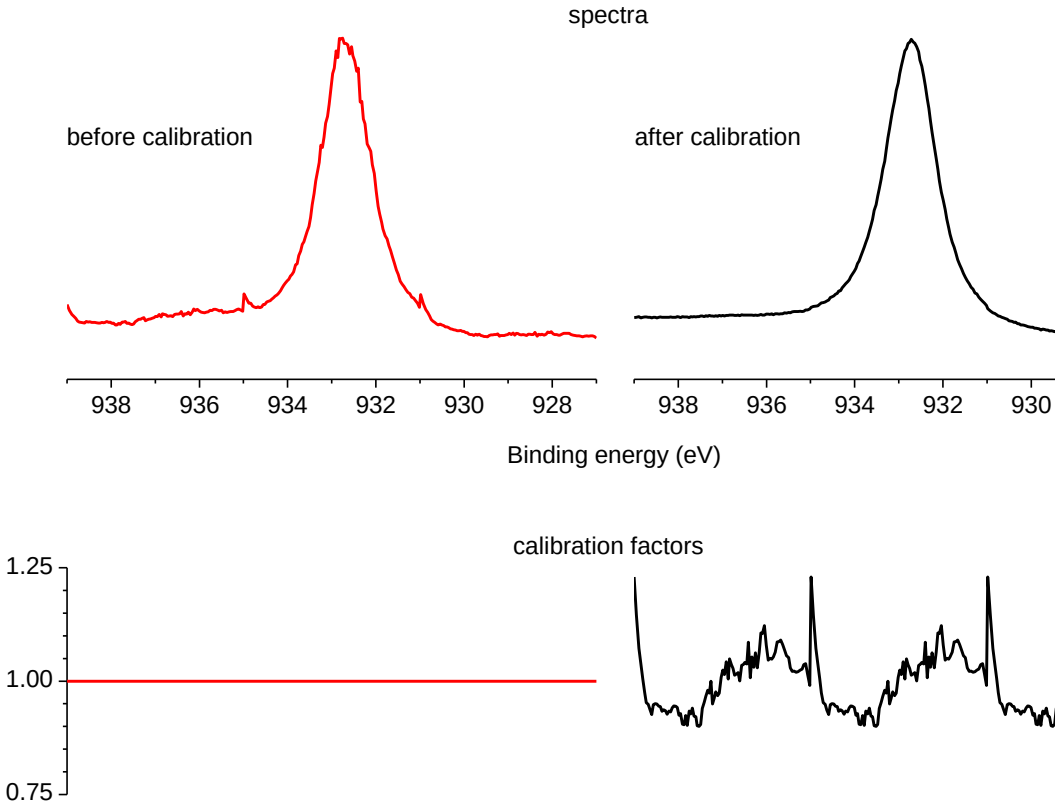
In KolXPD there are two important differences with respect to the SFAT mode in SpecsLab2:

- Broader choice of number of snapshots:
  the energy range in KolXPD does not have to be strictly multiple of 0.2*Epass. In the following example we show the situation equivalent to the one in 3.1.2 measured again by the MCD9 detector. The parameters were dwell time 500 ms (to have an equivalent statistics; before we had 100 ms dwell and 5 sweeps) and 10 snapshots (in order to have an average energy step 0.1 eV on the peak). The result is shown in the figure:



  One can see that if there are more than necessary to cover the energy range (minimum is 5*energy range/Epass, i.e. 5*12/20=3 in this case) the snapshots are equidistantly shifted in energy, therefore the resulting energy step is not equidistant; the points are more dense in the centre of the energy window and less near the its limits. For spectroscopy it may be fine as the more useful information (narrow features) is usually located in the centre while the borders represent only a broad background shape.
  The acquisition of the shown example takes 50 s which half of the time needed in the Standard measurement mode (see 3.1.2) for the same signal-to-noise ratio of the peak (and even less than those theoretical 60 s because some points near the limits are omitted).
  In the case of the 1D-DLD detector the number of separate channels is so high that it becomes almost ambiguous choice if better statistics is gained by higher dwell times or by higher number of snapshots, as the average energy step is usually sufficiently low in all cases.

- Channel gain calibration:
  As shown in the example 3.1.2 every single channel (of 9 or 100 depending on the detector) may have different sensitivity. It is not important when the user is interested only in the total intensity of the spectrum independently on its shape (e.g. in NEXAFS or XPD studies) but for the peak shape analysis it must be taken into account. SpecsLab2 uses the intensity factors from the calibration but these values may depend on all acquisition parameters and therefore be outdated. Contrary to it, KolXPD permits to perform a fast calibration at any time (and it performs it automatically before Photon energy, Angular and Sequence scans, see 3.2-3.4, respectively). The intensity calibration is simply done by running the same region once in the Standard measurement mode, after that the calibration factors are used for all following acquisition in the Smart mode.
  The calibration factors can be shown by clicking on the "View Channel Gain Calibration" button in the Analyzer settings panel (see 2.5.4).
  An example of the 1D-DLD calibration result is shown in the following figure on the peak acquired with the 1D-DLD detector by 3 non-overlapping snapshots (Epass = 20 eV so each snapshot is 4 eV wide). In the left part before calibration (calibration factors are all set to 1 by default, i.e. equal sensitivity of each of 100 channels), in the right part the channel gains are calibrated (they vary by ± 25%).



The comparison of both measurement modes is in the following table:

measurement mode	**Standard**	**Smart**
useful for	XPS, UPS	XPD, NEXAFS
speed	slower	faster
"waste"	0.4*Epass	none
energy step	constant	variable

calibration needed	only energy	energy and intensity
wrong calibration causes	broader peaks	very distorted peak shapes

3.1.4 Multiple region acquisition

KolXPD has not yet fully implemented the batch acquisition of several regions one after another as it in SpecsLab2 where regions can be easily added to/removed from the "to acquire" queue. However, also in KolXPD there is a way to acquire several regions one after another. They can differ in any acquisition parameters in the X-data range and Analyzer settings panels, typically photon energy, energy range, Epass and number of sweeps, but all others are possible (we remark that changing the lens mode takes several seconds so use one for all regions if possible). For the acquisition put all desired regions in one folder (for arrangement of the items in the tree see 2.4.2), click on the folder in the tree and press  in the Button bar. The regions will be acquired exactly as ordered in the folder.

3.2 Photon energy scan (3D data: hv – cps – KE/BE)

3.2.1 General remarks

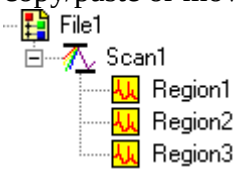
In this type of scan KolXPD automatically tunes the monochromator to the photon energy in the desired range and in each point it acquires one or more equal regions of the selected parameters, so it is useful for any type of measurements dependent on the used photon energy. Such scan can be used e.g. for the calibration of the monochromator on a reference sample, when the user is looking for the optimal photon energy (in order to maximize the signal as photon flux and cross sections may vary, minimize the contribution of the possibly disturbing core-levels, Auger or higher-order peaks overlapping the spectrum etc), perform resonant photoemission, band mapping, energy-resolved photoelectron diffraction or photoabsorption experiments. The examples together with some parameters are listed in the following table:

Purpose	**Scanned parameter**	**Measured region**	**Energy axis in region**	**Measuren mode**
monochromator calibration	photon energy, PM, PG, Cff	reference peak or Fermi level	Binding	Standard
looking for optimal photon energy	photon energy	desired peak or valence band	Binding	Standard
resonant photoemission	photon energy	desired peak or valence band	Binding	Standard
band mapping	photon energy	valence band	Binding	Standard
energy-resolved XPD	photon energy	desired peak	Binding	Smart
XAS, NEXAFS	photon energy	secondary electron or Auger peak	Kinetic	Smart

PM and PG scanning can be possibly used also for narrow scans of photon energy (in broader range the photon resolution and the beamline transmission may get worse).

For the tuning of the photon energy the communication between KolXPD and the monochromator must be properly set and working, as described in 1.4.5. The monochromator window is used the same way as described in 3.1.1.

To perform the photon energy scan simply create the corresponding item in the Tree using  in the Button bar (see 2.3) (or copy/paste or move it from any previous experiment). By default the newly created Photon energy scan it will contain one region, more of them can be added using , copy/paste or move), see the example in the following figure:



3.2.2 Region parameters

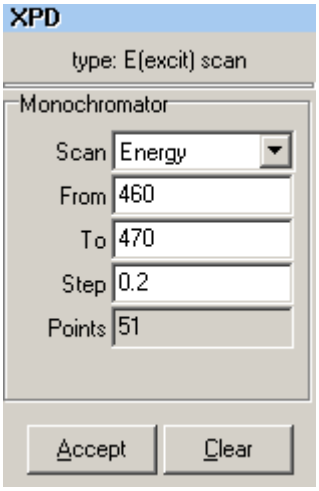
The acquisition parameters of the region(s) can be freely set as described in 3.1.2-3.1.3, therefore they can be different for every region. However, there are several important notes:

- Excitation energy setting:
  For the scan in photon energy in is not important to set the excitation energy in the X-data range panel (2.5.3, 3.1.2) as it will be overridden in each point by the actual value anyhow. Only in the rather special case of scan in Cff (see the table in 3.2.1), where the photon energy is constant, KolXPD will take this value into account.
- Lens mode setting:
  Analogously to what was described in 3.1.4 it is possible to set for each region even a different Lens and detector parameters in the Analyzer settings panel (2.5.4, 3.1.2) but it is not recommended because switching these parameters during the scan may take several seconds and therefore cause delays.
- Channel gain calibration in the Smart mode:
  If there are any regions set to be acquired in the Smart mode KolXPD will automatically perform the channel gain calibration (see 3.1.3) by acquiring these regions **once** (before the scan) in the Standard mode using the parameters in the Analyzer settings panel, section Measurement mode/Standard. If you for any reason desire to avoid this calibration set the number of sweeps to **0** before switching from Standard to Smart.

To check the correctness of every region's acquisition parameters and/or the speed of acquisition just select it in the Tree and press , it will not start the Photon energy scan but only the region as described in 3.1.2 or 3.1.3.

3.2.3 Scan parameters

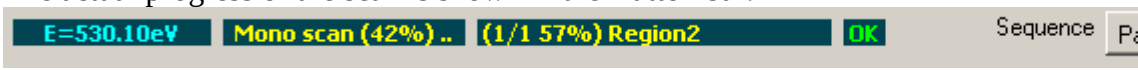
The parameters of the Photon energy scan are obviously the parameters of the tuning of the monochromator. The corresponding panel is shown in the following figure:



The most typical is the scan in energy as shown. The user needs to set the upper and lower limits and the step, KolXPD then calculates the number of points to be measured as the rounded value of *(To–From)/Step+1*, therefore if *To–From* is not divisible by *Step* the *To* point cannot be included and the whole scan finishes at *To–Step* or *To+Step*.
After clicking on Accept the editable fields are locked, if the values do not comply with the limits set in the configuration file (see 1.4.5) they will be automatically adjusted. In order to be sure check that they are as desired. For unlocking the fields click on the Clear button. Use the same button also for clearing the scan from previously acquired data.

3.2.4 Running the scan

When all parameters are set and accepted the scan can be started by clicking on  in the button bar. First, the channel gain calibration is performed for all regions to be acquired in the Smart mode (if any), then the monochromator is tuned to the *From* value, then all regions are acquired at this photon energy, then the monochromator is tuned to the *From+Step* value, all regions are again acquired and so on until the last point is acquired.
The actual progress of the scan is shown in the Button bar:

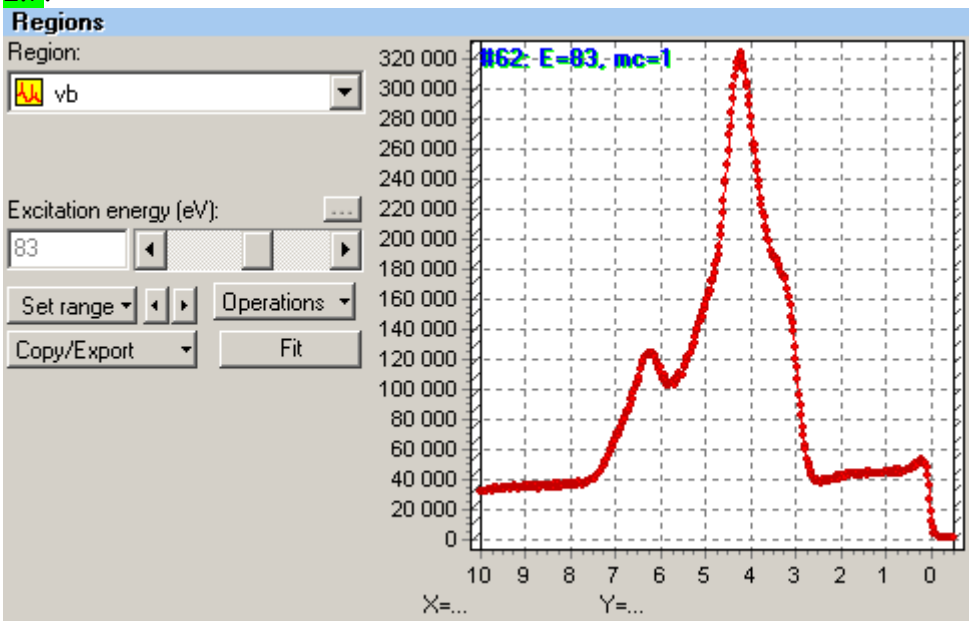


namely the actual energy of the analyzer (cyan), current status of the scan (points acquired/total points, percentage, yellow), current status of the region acquisition (current sweep/total sweeps, percentage, region title, yellow), status (green if OK and red in the case of error) and several other buttons. They permit to pause the scan after the current point using the Pause button (which is different from  in the Button bar that pauses immediately), and then select the next point to continue by using the arrow next to it. Such action permits to skip some points or repeat those that were acquired incorrectly (e.g. if the synchrotron beam was unstable). The four checkboxes allow the select if the corresponding panels will be updated automatically their view in each point of the scan. [Podle mě tahle věc je zbytečná a nejasná a mohla by se vyhodit.]

By clicking on  and  in the Button bar the spectra are saved in each point to the autosave.xpd file and the analyzer will be disconnected at the end of the scan, respectively.

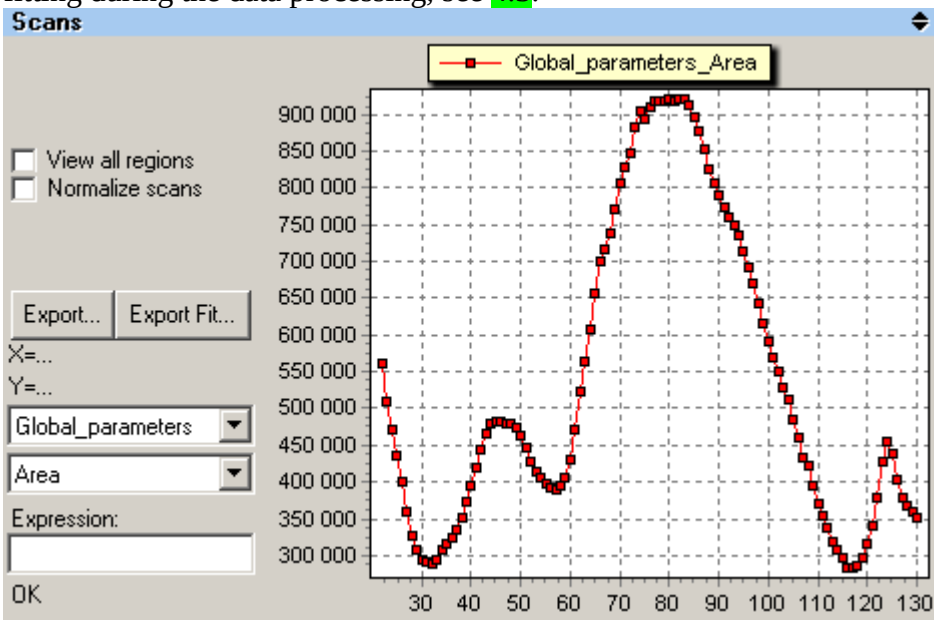
3.2.5 Regions panel

This panel shows the actually acquired spectrum (intensity vs. binding or kinetic energy) of the selected region together with the one acquired in the previous step (if available). The details about the options in this panel are described in the Data processing section (see 4.3) but some of them are already available during the acquisition, mainly selecting the region (if more than one are being acquired), browsing the data acquired at different photon energies and selecting the spectra range for the Scans panel as described in 2.7.



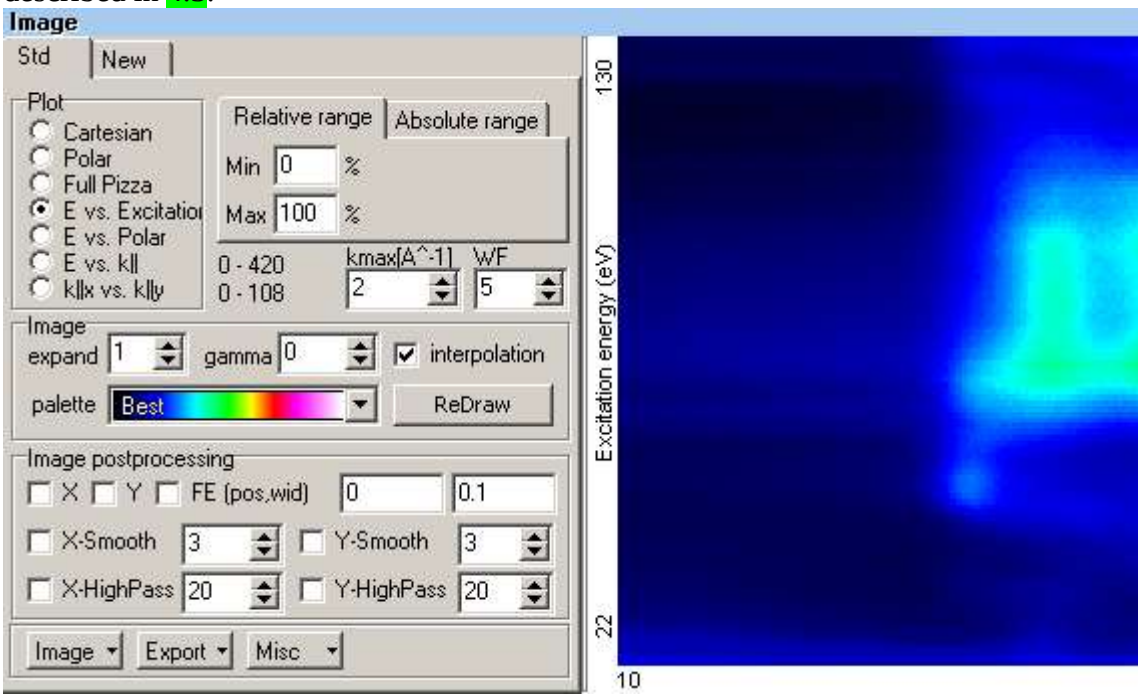
3.2.6 Scans panel

During the photon energy scan acquisition the user can display the evolution of the selected parameter from the region and range displayed in the Regions panel (or all available regions at the same time, also normalized if needed) vs. photon energy. The parameters readily available during the acquisition are called Global parameters and include mesh current, spectrum area as is or after the subtraction of a linear background, and these areas divided by the mesh current. More parameters are available after the peak fitting during the data processing, see 4.3.



3.2.7 Image panel

Although the main purpose of the Image panel is to display a graphical representation of the angular scans, some options can be useful also for the photon energy scans and may be available already during the acquisition. In the following example we show the intensity plot with binding energy on the horizontal axis and photon energy on the vertical axis. More details are described in 4.3.



3.3 Angular scan (3/4D data: θ/φ – cps – KE/BE)

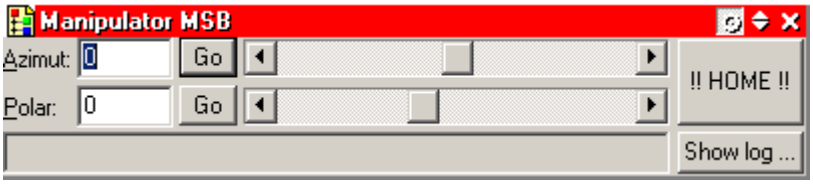
3.3.1 General remarks

In this type of scan KolXPD automatically moves one or two stepping motors of the manipulator, usually controlling the rotation around the sample normal (azimuth) and the polar angle. In each point it acquires one or more equal regions of the selected parameters so it is useful for any type of angle-resolved measurements such as X-ray photoelectron diffraction, angle-resolved ultraviolet photoelectron spectroscopy or band mapping. Except for some differences the acquisition procedure is very similar that of Photon energy scans describer in 3.2.

For Angular scans in might be necessary to improve the angular acceptance of the analyzer entrance optics, e.g. by using the iris aperture installed in the Specs Phoibos 150 analyzers or by selecting the appropriate lens mode.

3.3.2 Manipulator window

For the tuning of the photon energy the communication between KolXPD and the manipulator must be properly set and working, as described in 1.4.5. The monochromator window is very simple, it contains independent controls of both axes, the HOME button to move to the 0,0 position (normal emission) and the Show log... button to see the logged communication:



To perform the photon energy scan create the corresponding item in the Tree using  in the Button bar (see 2.3) (or copy/paste or move it from any previous experiment) similarly to 3.2.1. By default the newly created Angular scan it will contain one region, more of them can be added using , copy/paste or move.

3.3.3 Region parameters

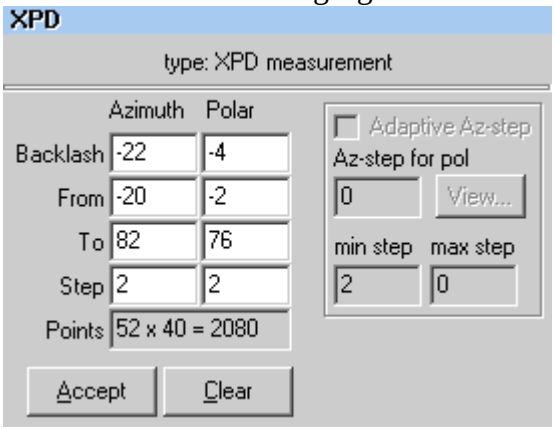
Analogously to 3.2.2 The acquisition parameters of the region(s) can be freely set as described in 3.1.2-3.1.3, therefore they can be different for every region. The latter two important notes described in 3.2.2 are valid also here:

- Lens mode setting:
  It is possible to set for each region even a different Lens and detector parameters in the Analyzer settings panel (2.5.4, 3.1.2) but it is not recommended because switching these parameters during the scan may take several seconds and therefore cause delays.
- Channel gain calibration in the Smart mode:
  If there are any regions set to be acquired in the Smart mode KolXPD will automatically perform the channel gain calibration (see 3.1.3) by acquiring these regions **once** (before the scan) in the Standard mode using the parameters in the Analyzer settings panel, section Measurement mode/Standard. If you for any reason desire to avoid this calibration set the number of sweeps to **0** before switching from Standard to Smart.

To check the correctness of every region's acquisition parameters and/or the speed of acquisition just select it in the Tree and press , it will not start the Angular scan but only the region as described in 3.1.2 or 3.1.3.

3.3.4 Scan parameters

The fundamental parameters of the Angular scan are those of the polar and azimuth rotation angle of the sample manipulator. The corresponding panel is shown in the following figure:



The user needs to set the upper and lower limits and the step, and the absolute backlash (in the shown example it is 2 degrees below the starting value). KolXPD then calculates the number of points to be measured as the rounded value of *(To–From)/Step+1*, therefore if *To–From* is not divisible by *Step* the *To* point cannot be included and the whole scan finishes at *To–Step* or *To+Step* in both axes. If only one axis is to be scanned set the on other one *Backlash*, *From* and *To* to the same value so the scanning is avoided.
After clicking on Accept the editable fields are locked, if the values do not comply with the limits set in the configuration file (see 1.4.5) they will be automatically adjusted. In order to be sure check that they are as desired. For unlocking the fields click on the Clear button. Use the same button also for clearing the scan from previously acquired data.
what to do when one axis is missing

3.3.5 Running the scan

When all parameters are set and accepted the scan can be started by clicking on  in the button bar. First, the channel gain calibration is performed for all regions to be acquired in the Smart mode (if any), then the manipulator rotates the sample to the *Backlash* angles, then to *From* angles and all regions are acquired at this position and so on. The azimuth rotation is the outer loop of the cycle in order to minimize the necessary movement of the less robust mechanism (moving parts in vacuum). The inner loop is polar rotation so at every azimuth angle all desired polar angles are acquired one after another.
The actual progress of the scan is shown in the Button bar:

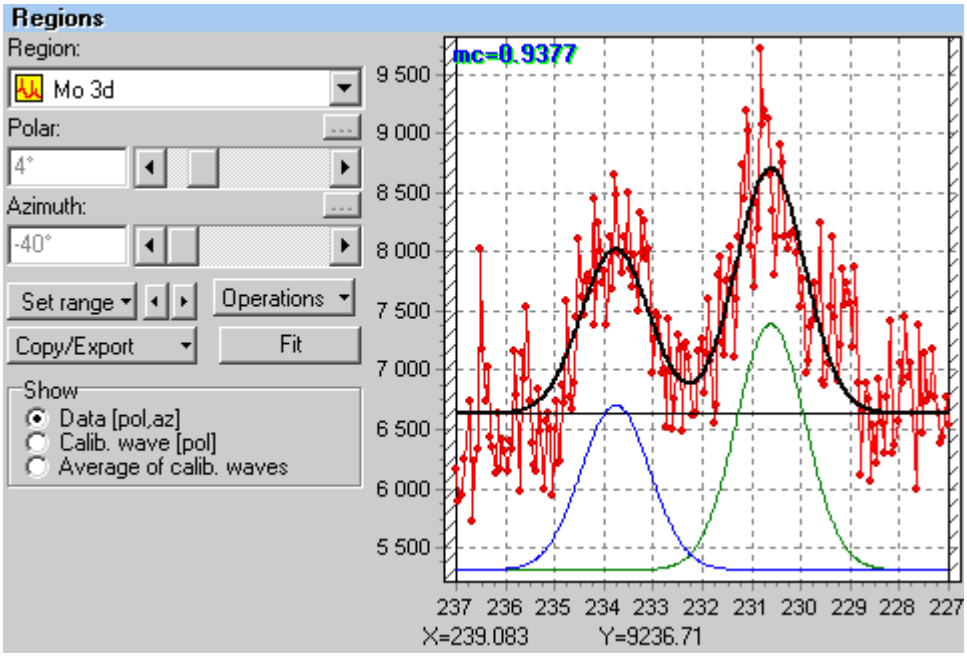


namely the actual energy of the analyzer (cyan), current status of the scan (points acquired/total points, percentage, yellow), current status of the region acquisition (current sweep/total sweeps, percentage, region title, yellow) and the status (green if OK and red in the case of error). The four checkboxes allow the select if the corresponding panels will be updated automatically their view in each point of the scan. [Podle mě tahle věc je zbytečná a nejasná a mohla by se vyhodit.]

By clicking on  and  in the Button bar the spectra are saved in each point to the autosave.xpd file and the analyzer will be disconnected at the end of the scan, respectively.

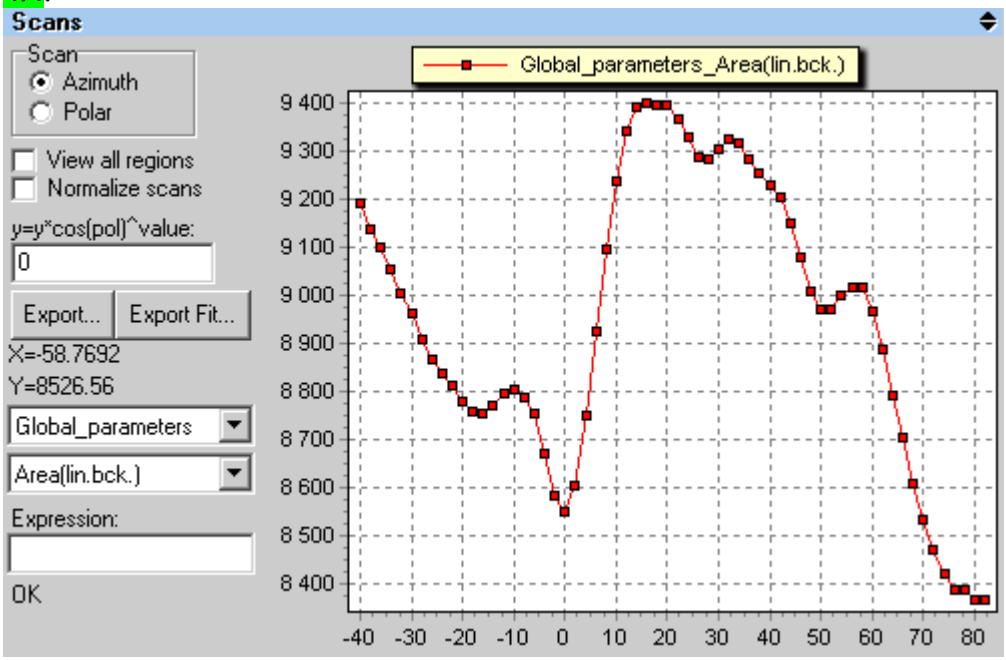
3.3.6 Regions panel

This panel shows the actually acquired spectrum (intensity vs. binding or kinetic energy) of the selected region together with the one acquired in the previous step (if available). The details about the options in this panel are described in the Data processing section (see 4.4) but some of them are already available during the acquisition, mainly selecting the region (if more than one are being acquired), browsing the data acquired at sample angles and selecting the spectra range for the Scans panel as described in 2.7.



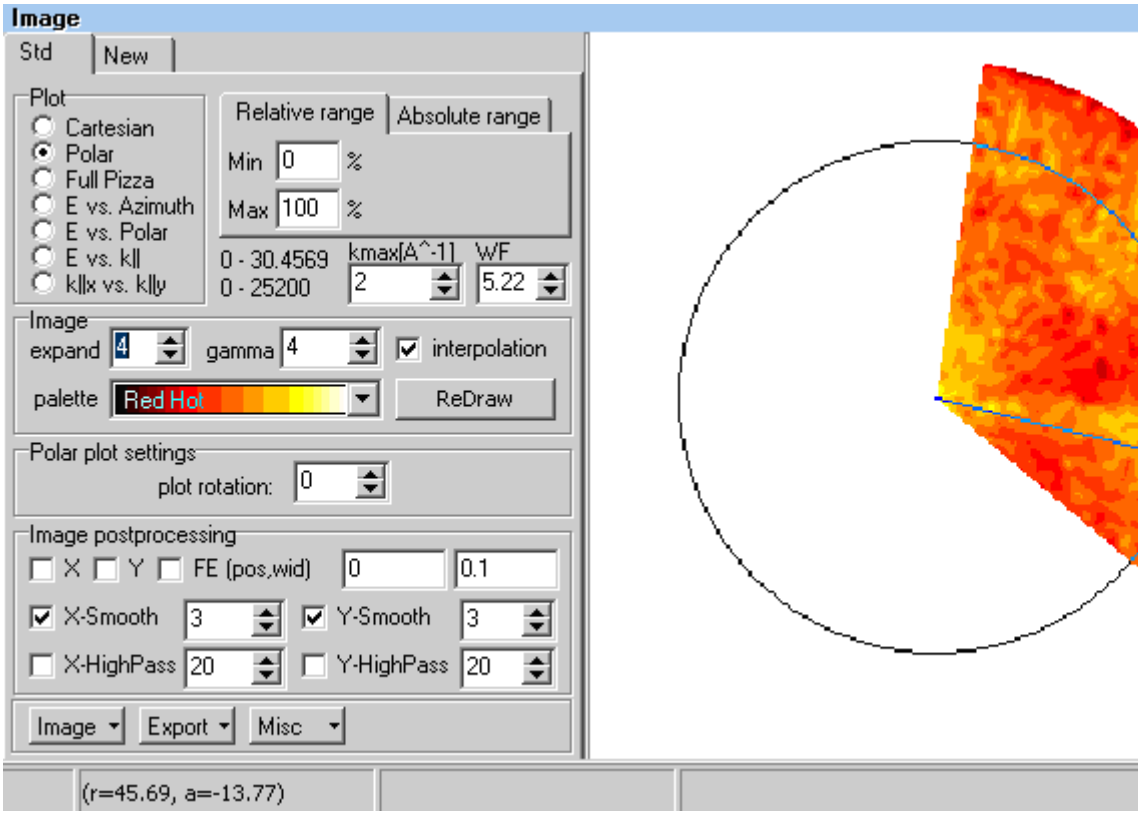
3.3.7 Scans panel

During the Angular scan acquisition the user can display the evolution of the selected parameter from the region and range displayed in the Regions panel (or all available regions at the same time, also normalized if needed) vs. azimuth or polar angle. The parameters readily available during the acquisition are called Global parameters and include mesh current (if synchrotron radiation is used), spectrum area as is or after the subtraction of a linear background, and these areas divided by the mesh current. More parameters are available after the peak fitting during the data processing, see 4.4.



3.3.8 Image panel

This panel displays a graphical representation of the angular scans, most typically the polar graph of the acquired photoelectron peak intensity in XPD, as shown in the following example. More details are described in 4.4.



3.4 *Sequence scan (3D data: time – cps – KE/BE)*

Sequence scan, no idea how it works

4 Data processing

4.1 Obtaining data

4.1.1 Acquisition

see 3

4.1.2 Open SpecsLab2 xml and xy files

describe MCD/Sweeps button

4.1.3 Open other files

describe Import dialog

4.1.4 Import from clipboard

see 4.1.3

4.1.5 Import VG 2D-detector data

http://eshop.kolibrik.net/en/kolxpd/manual/11-importing-2d-data-files

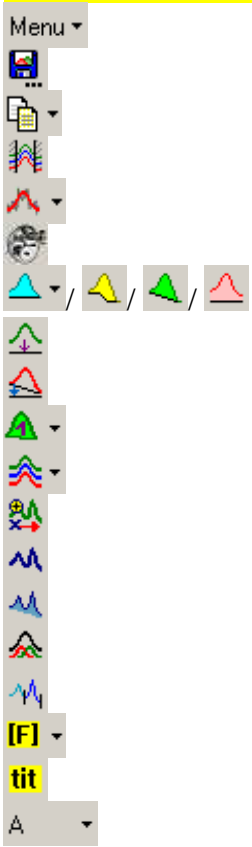
4.1.6 Convert 2D set to 3/4D

http://eshop.kolibrik.net/en/kolxpd/manual/13-creation-of-parameter-resolved-experiment-items-from-set-of-spectra

4.2 Region processing (2D data: cps – KE/BE)

4.2.1 Display

describe multiview (reference to 2.7 for graph operations).





4.2.2 Region parameters

see 2.5.3, 2.5.4 for cross section etc and "Set to all items..." dialog in 2.4.3

4.2.3 Editing

Edit table items, Processing panel in 2.5.6

4.2.4 Fitting

fitting module, background, curve types, fitting, fixing, constraints...
http://eshop.kolibrik.net/en/kolxpd/manual/12-fitting-with-independent-parameters

4.2.5 Export fit parameters

describe fully the Export dialog

4.2.6 Export fitted spectra

similar to 4.2.5

4.3 Photon energy scan processing (3D data: hv – cps – KE/BE)

4.3.1 Display

"Scans" window

4.3.2 Editing

"Operations..." dialog

4.3.3 Fitting

see 4.2.4 , extend to Copy prm and Copy all

4.3.4 Export fit parameters

see 4.2.5

4.4 Angular scan processing (3/4D data: θ/φ – cps – KE/BE)

4.4.1 Display

"Image" window

4.4.2 Editing

"Operations..." dialog

4.4.3 Fitting

see 4.2.4 , extend to Copy prm and Copy all

4.4.4 Export image

describe the export

4.5 Sequence scan processing (3D data: time – cps – KE/BE)

4.5.1 ???

???

4.5.2 ???

???

5 Troubleshooting

6 Index

alphabetical index of keywords

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